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FINAL REPORT

PROJECT NO. E–20–604

MATHEMATICAL MODELING OF AQUATIC DISPERSION OF EFFLUENTS

By

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Morris L. Maslia

Prepared for

HEALTH AND SAFETY DIVISION
OAK RIDGE NATIONAL LABORATORIES
OAK RIDGE, TENNESSEE

Through The

BIOLOGY DEPARTMENT
EMORY UNIVERSITY

July, 1980

GEORGIA INSTITUTE OF TECHNOLOGY

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ATLANTA, GEORGIA 30332

1980

MATHEMATICAL MODELING OF AQUATIC

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Health and Safety Division
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July, 1980

PREFACE

This final report is the result of a six-month contract between the Health and Safety Division of the Oak Ridge National Laboratories through Emory University Biology Department and the Georgia Institute of Technology. The study was conducted in School of Civil Engineering, Georgia Institute of Technology, Atlanta, Georgia.

Of considerable aid in the initial conception and planning of the study was Dr. P. G. Mayer, School of Civil Engineering, Georgia Institute of Technology. Mr. M. Maslia, Graduate Assistant, helped the principal investigator in several phases of the study including data analysis and the preparation of some of the computer codes. The project was directly administered by Dr. H. L. Ragsdale, Biology Department, Emory University, Atlanta, Georgia.

The purpose of this study was to investigate the possibilities of preparing a user-oriented computer model to predict mass transport characteristics of natural rivers, for a given site, with minimum available physical parameter data. Due to the existing time limitations, this project could only constitute an initial step in a series of such modeling studies, and should be considered as such. At this time the accumulated know-how and the results obtained clearly indicate that it is possible to generate useful regional computer models which analyze the mass transport problem for river systems in one and/or two dimensions. The input data required in such a regional model will be the minimum available input data both in terms of physical parameters and kinematic variables of the problem.

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1.0 INTRODUCTION

In the course of time a number of methods and computational procedures have been developed to investigate and to predict mass transport in natural rivers. A literature review in this research area indicates that several Environmental Transport Models with varied degrees of complexity and different simulation objectives are available. A recent report by Little and Miller (1979) provides a rather complete listing of such studies as well as a critical review of them. One major problem with these models is that it is often very difficult to implement them. The reason for this is in part the inaccessibility of the generated computer code and in part, the specific, problem-oriented design employed. It is well known that model design, almost by definition, is a pragmatic process - the simulation objectives determine the basic form, usability, and generality of the model. An investigation of the various available models, approved by U.S. Nuclear Regulatory Commission Regulatory Guide 1.113 (1977), which focuses on their usability and applicability in predicting the transport of a quantity of pollutant in a surface water environment following an accidental spill, clearly indicates the necessity of user-oriented, well documented computer models. Thus, the present study is an initial step toward the goal of preparing and documenting a user-oriented computer model which will be available for use in cases of emergency, to predict the mass transport of pollutants in natural rivers with minimum available input data.

Although the short duration of the study imposed considerable restrictions on the findings that could be obtained at this stage, this initial work proved helpful with regard to feasibility assessment. Following an accidental discharge of radioactive materials or chemicals into a river, whatever the cause of the accident, it is important to provide immediate information to water users downstream on the expected pollutant concentration in the river at various times and locations. A well documented regional computer model may be very useful in such cases of emergency. Initial estimates of the magnitude of the problem as it varies through time can be obtained quickly by employing a model of this kind. At this time it is clear that such regional computer models which analyze the mass transport problem for river systems, in one and/or two dimensions, with minimum available input data both in terms of physical parameters and kinematic variables of the problem, can be generated.

Model accuracy and reliability are two of the more important aspects of numerical modeling which should not be overlooked. If a numerical model is to be accepted as a reliable predictive tool, the numerical error bounds generated should be within acceptable limits, and the model should be validated regionally using available data. Proceeding in this direction, much of the recent work done in water quality modeling has been oriented towards improvement of models -- towards incorporating better numerical solution techniques, the accuracy of which surpass by far the availability and accuracy of the field parameter data that have to be used with such models. Scarcity of such data, especially in surface water quality modeling, is well known to researchers and engineers working in this field.

Currently there is some disagreement among researchers as to whether higher priority should be placed on still further developments in model sophistication or on parameter prediction to improve accuracy. Naturally, improved sophistication of models is associated with increases in number of model parameters. Since it is likely that many of the additional parameters would be defined only in qualitative terms, a relatively more sophisticated model can be less reliable than a simpler version. On the other hand, however, some systems and some physical phenomena are so complex in nature that there is often little reason to believe that good simulations are possible with simplified representations. In such cases the need for more detailed and realistic models is clear. A simple and crude example can be found in the case of transport models for river systems. Given the current understanding and knowledge on turbulence characteristics, secondary currents, roughness concepts and sediment transport characteristics of natural rivers, it may be overly ambitious to attempt to develop a three-dimensional transport model for a river system just because it is possible numerically. Going to the other extreme, if in order to simplify such a model, that is, in order to reduce the model dependence to field parameters, one ignores the diffusive transport terms keeping the convective transport terms in the analysis, the reliability of the model becomes questionable, at least for certain problem types like accidental spills of pollutants or daily cyclic variation of spills, as is the case in sewage output. In relation to the production of user-oriented models, the optimum solution lies between these two extremes.

In an attempt to achieve this goal, an initial effort is made in this study to analyze the one-dimensional mass transport equation, with the possibility of generating some default values for field parameters like the longitudinal diffusion coefficient and decay constants for several radioactive materials. Thus, the purpose of the present study is the generation of a computer model to analyze mass transport phenomena in a river. This model will be the first step in an overall study of regional models. At this step, no attempt is made to generate default values to predict regional hydrogeologic and local kinematic parameters for river systems. That problem will be considered in a later stage of the study.

Given the boundaries of the task as defined above, a numerical computer model is developed using the finite element method. The generated model includes some routines to predict the longitudinal diffusion coefficient, given some kinematical constants. Also, decay constants are generated, given the specification of the radioactive material under study. Several analytical solutions for the mass transport equation are reviewed, and computer programs for such analytic solutions are presented as a supplement, in addition to the finite element model.

2.0 MATHEMATICAL MODEL

Transport of pollutants in natural rivers is a complex phenomenon, especially if an effort is made to cover all aspects of it. In an industrialized society, a great variety of pollutants can get mixed into surface waters. Dissolved matters such as chemicals, radioactive materials, and salt, solid matters such as sediments, and temperature gradients introduced by power plants may roughly describe the basic sources of pollution. Different models are needed to describe the transport characteristics of different pollutants. Thus, the choice of type of pollution is the first step to be considered. The stage of pollution transport is another variable, since mathematical models describing initial mixing zones are considerably different than mathematical models to be used for well mixed zones. The third variable is the choice of model dimensions. Given the present know how in numerical methods, it is tempting to develop a three-dimensional model, with the asumption that the parameters needed in such a model are readily available. Thus, determination of physical and kinematic parameters is the fourth complexity encountered in the modeling of transport of pollutants in natural rivers. Parameters like longitudinal and transverse diffusion coefficients, decay of organic matter and other chemicals, heat transfer to atmosphere through water surface, erosion and deposition of sediments in natural environments have been studied by many researchers in the field, with no universal description of the phenomena involved. Keeping these complexities in mind, the boundaries of the model developed for this project are summarized below, following the guidelines and limitations described in detail in Section 1.

2.1 Transport Model

A one-dimensional model is used to describe the longitudinal transport of pollutants in natural rivers. Such an analysis is very useful in the study of accidental spills of pollutants from nuclear power plants or daily cyclic variations of output from sewage treatment plants. It is assumed that low concentration solutions of matter are transported with mean river velocity. Such an assumption helps to avoid the study of density currents which result in all cases of high concentration transport. It is assumed that dispersion is caused by uneven distribution of flow over a cross section, and dispersion effects due to overbank storage, tidal flows, and action of wind and waves are ignored. Further, the model does not describe the initial mixing stage of pollutant transport phenomena. Thus, transport of matter by such a mixing process including the molecular and turbulent diffusion effects may be lumped into one term if such a process can be regarded as a continuous exchange of unit volumes of water with concentration C_1 and C_2 ($C_2 > C_1$) over a distance ℓ (mixing length) with a velocity v'. This description of diffusive transport may be given mathematically as,

$$M_1 = - D\frac{\partial C}{\partial x} \qquad (2.1)$$

where,

$$D = v'\ell \qquad (2.2)$$

and the negative sign is due to the direction of transport which is towards the area of lower concentration. Transport due to convection by mean velocity, on the other hand, can be described as,

$$M_2 = \bar{u}C \qquad (2.3)$$

Thus, as a first approximation, the total transport may be given as,

$$M = \bar{u}C - D\frac{\partial C}{\partial x} \qquad (2.4)$$

In Equation (2.4), $\bar{u}$ describes a cross sectional mean velocity in the direction of flow and D is the longitudinal diffusion coefficient which is discussed in more detail in the following section.

In addition to diffusive and convective transport of matter, the continuity equation should be satisfied to describe the transport phenomena properly. Considering a control volume approach (see Figure 1), the gradient of transport across the faces of the control volume can be given as,

$$I_1 = \frac{\partial M}{\partial x} \qquad (2.5)$$

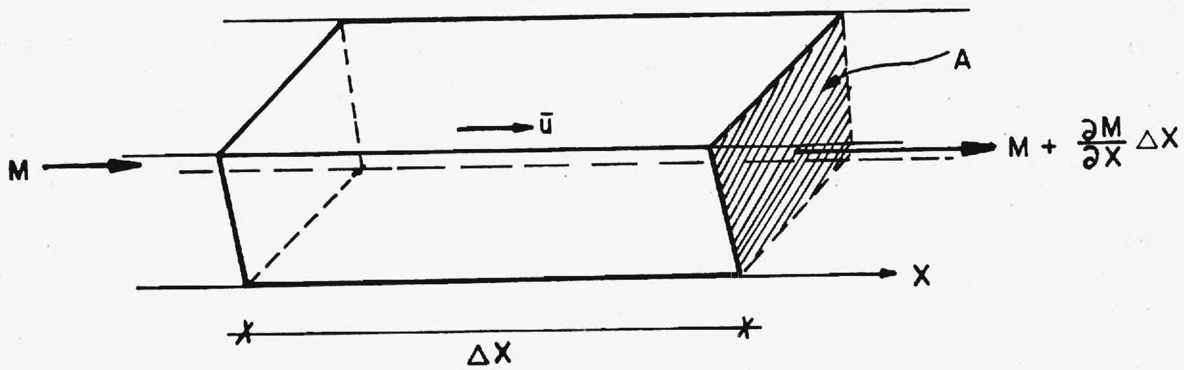

FIGURE 1. Control Volume

The change of concentration over time in the control volume can be given as,

$$I_2 = \frac{\partial C}{\partial t} \qquad (2.6)$$

and further, decay for non-conservative substances or uptake in case of biological interactions can be represented by,

$$I_3 = KC \qquad (2.7)$$

where K is a first order decay constant. Summation of Equations (2.5), (2.6), and (2.7) should be zero to satisfy continuity. Thus,

$$\frac{\partial M}{\partial x} + \frac{\partial C}{\partial t} + KC = 0 \qquad (2.8)$$

Integrating Equations (2.4) and (2.8) over a cross-section A results in,

$$\bar{M} = A\ \bar{u}\ \bar{C} - AD\frac{\partial \bar{C}}{\partial x} \qquad (2.9)$$

and,

$$\frac{\partial \bar{M}}{\partial x} + \frac{\partial A\bar{C}}{\partial t} + AK\bar{C} = 0 \qquad (2.10)$$

Substituting (2.9) into (2.10), one may write,

$$\frac{\partial}{\partial t}(A\bar{C}) + \frac{\partial}{\partial x}(A\bar{u}\bar{C}) - \frac{\partial}{\partial x}(AD\frac{\partial \bar{C}}{\partial x}) + AK\bar{C} = 0 \qquad (2.11)$$

where A is the cross-sectional area of the river, K is the first order decay coefficient, $\bar{C}$ is mean concentration, $\bar{u}$ is mean velocity, D is the longitudinal dispersion coefficient, and (x) and (t) are space and time coordinates. The equation of continuity for river flow can be written as,

$$\frac{\partial A}{\partial t} + \frac{\partial}{\partial x}(A\bar{u}) = 0 \qquad (2.12)$$

Combination of Equations (2.11) and (2.12) yields,

$$\frac{\partial \bar{C}}{\partial t} + \bar{u}\frac{\partial \bar{C}}{\partial x} - \frac{1}{A}\frac{\partial}{\partial x}(AD\frac{\partial \bar{C}}{\partial x}) + K\bar{C} = 0 \qquad (2.13)$$

Equation (2.13) will be used to describe the time dependent one-dimensional transport of pollutants in natural rivers in this study. The limitations of the above equation and the one-dimensional approach are described in several places in this report. The reader is referred to Fisher (1979) and Bird (1960), for further details.

The general one-dimensional convective-dispersion equation given by (2.13) is of parabolic type if all terms are important. However, in certain situations where one mechanism is more important than the other, a classification can be made according to the relative importance of diffusion versus convection.

Defining some characteristic diffusion coefficient $\bar{D}$, characteristic velocity U and length L, the relative importance of diffusion versus convection is measured by the ratio of the quantities ($A\bar{C}U$) and ($\bar{D}A\bar{C}/L$). This enables one to define a generalized Reynolds or Peclet number ($UL/\bar{D}$) as the ratio of convective to diffusive transport. If ($UL/\bar{D} \ll 1$) convection terms can be neglected, and if ($UL/\bar{D} \gg 1$) diffusion terms can be neglected. In all other cases, both terms are significant in the overall mass transport analysis. When diffusion effects are negligible, that is for ($UL/\bar{D} \to \infty$), Equation (2.13) becomes of hyperbolic nature, while for other cases the transport equation is of parabolic type. In the absence of convective effects, the steady state form of Equation (2.13) is of elliptic type. The presence of the convective terms in a general unsteady problem does not change the parabolic nature of the equation, but these terms generate the non-symmetric character of the partial differential equation. This non-symmetric character of the partial differential equation constitutes one of the main problems in the numerical discretisation of the convective-diffusion equation, especially for high values of UL/D.

Although the complications due to density differences, sediment transport and tidal flow are eliminated in the mathematical model given above, a simple analytical solution of Equation (2.13) as such is not possible. However, it is possible to simplify Equation (2.13) further to describe some analytical solutions depending on the boundary and initial conditions for different problems. The rest of this section is devoted to a review of analytical solutions possible for simplified forms of the one-dimensional mass transport equation. User-oriented computer programs are presented for some of these solutions in Appendix I to further supplement the reader with available tools of mass transport analysis.

2.2 Review of Analytical Solutions

Equation (2.13) can be simplified further if one assumes constant channel cross section and steady flow conditions. With these assumptions, for a non-conservative substance, Equation (2.13) yields,

$$\frac{\partial \bar{C}}{\partial t} + \bar{u}\frac{\partial \bar{C}}{\partial x} - D\frac{\partial^2 \bar{C}}{\partial x^2} + K\bar{C} = 0 \qquad (2.14)$$

Equation (2.14) is of parabolic type. To solve this equation, an initial condition and two boundary conditions are required. The initial condition describes the concentration distribution over the whole area at the initial time t = 0.

$$\bar{C}(x,0) = f(x) \qquad (2.15)$$

Some typical examples of boundary conditions that can be used in solution of Equation (2.14) can be given as:

a) The concentration at location x = a is a specified function of time or is given as a constant value, a Dirichlet boundary condition.

$$\bar{C}(a,t) = c_o(t) \qquad \text{or} \qquad \bar{C}(a,t) = c \tag{2.16}$$

b) There is no dispersive transport at the boundary x = a, a Neuman boundary condition.

$$\frac{\partial \bar{C}}{\partial x} = 0 \quad \text{at} \quad x = a \tag{2.17}$$

c) At infinity the concentration must vanish.

$$\lim_{x \to \infty} \bar{C}(x,t) = 0 \tag{2.18}$$

d) Supply of mass flux is specified at location x = a, a Mixed type boundary condition.

$$\lim_{x=a^-} [A\bar{u}\bar{C} - AD\frac{\partial \bar{C}}{\partial x}] - \lim_{x=a^+} [A\bar{u}\bar{C} - AD\frac{\partial \bar{C}}{\partial x}] = \bar{W} \tag{2.19}$$

where $\bar{W}$ is the supply of mass per unit of time at x = a. Given these boundary conditions analytical solutions to typical problems are described below:

A) If a mass of material, $\bar{W}$, is released instantaneously and uniformly over a cross section at time t = 0, the location of which is designated as the origin, with concentration being zero at an infinite distance downstream and with zero concentration distribution in the reach as an initial condition, then the solution of Equation (2.14) is given as,

$$\bar{C} = \frac{\bar{W}}{2A\sqrt{\pi D t}} \exp\left(\frac{-(x-\bar{u}t)^2}{4Dt} - Kt\right) \tag{2.20}$$

In this problem the mass $\bar{W}$ is released at t = 0 over the area A, located at x = 0. As the material moves downstream its concentration is decreased by the characteristic reaction coefficient, K, and its mass is spread downstream from its center of gravity with the net downstream velocity of the river.

B) If one ignores the reaction term and keeps the description of boundary conditions given above as is, then the analytical solution reduces to,

$$\bar{C} = \frac{\bar{W}}{2A\sqrt{\pi Dt}} \exp\left(\frac{-(x-\bar{u}t)^2}{4Dt}\right) \qquad (2.21)$$

C) If one describes the input of pollutants as a continuous flux of supply at the location x = 0 and the channel is infinite to both sides of the source, then the following initial and boundary conditions hold.

Initial condition: $\bar{C}(x,0) = 0$ (2.22)

Boundary condition one: $\lim_{|x|\to\infty} \bar{C}(x,t) = 0$ (2.23)

Boundary condition two: $\lim_{x=0^-} AD\frac{\partial \bar{C}}{\partial x} - \lim_{x=0^+} AD\frac{\partial \bar{C}}{\partial x} = \bar{W}$ (2.24)

Given a conservative pollutant, the solution to this case can be given as,

$$\bar{C}(\alpha,\beta) = \frac{\bar{W}}{2\bar{u}}\left[e^{4\alpha}\left\{\operatorname{erf}\left(\beta + \frac{\alpha}{\beta}\right) - \operatorname{sign}(\alpha)\right\} + \operatorname{erf}\left(\beta - \frac{\alpha}{\beta}\right) + \operatorname{sign}(\alpha)\right] \qquad (2.25)$$

where

$$\alpha = \frac{\bar{u}}{4D}x \quad , \quad \beta = \frac{\bar{u}}{2}\sqrt{\frac{t}{D}} \qquad (2.26)$$

and

$$\operatorname{erf}(y) = \frac{2}{\sqrt{\pi}}\int_0^y e^{-x^2}dx \quad , \quad \operatorname{sign}(\alpha) = \begin{cases} +1 & \alpha>0 \\ -1 & \alpha<0 \end{cases} \qquad (2.27)$$

D) Given Equation (2.14) the problem defined in the previous case can be extended to a non-conservative substance with continuous injection at x = 0 at a rate $\bar{W}$ (lb/sec), with downstream conditions and initial conditions defined as before. The following analytic solution can be given for such a case.

$$\bar{C} = \frac{W}{2\Omega} \exp\left(\frac{x\bar{u}}{2D}\right) \left\{ \left[\operatorname{erf}\left(\frac{x+\Omega t}{\sqrt{4Dt}}\right) \pm 1\right] \exp\left(\frac{x\Omega}{2D}\right) - \left[\operatorname{erf}\left(\frac{x-\Omega t}{\sqrt{4Dt}}\right) \pm 1\right] \exp\left(-\frac{x\Omega}{2D}\right) \right\} \tag{2.28}$$

where,

$$\Omega = \sqrt{\bar{u}^2 + 4KD} \tag{2.29}$$

and the minus sign applies to values of x>0 and positive sign applies to values of x<0.

E) In all of the solutions given above solution domains are assumed to be infinite. The following analytical solution can be described for a finite region for a conservative substance provided that initial and boundary conditions are described as,

Initial condition: $\bar{C}(x,0) = 0 \quad 0 \leq x \leq L$ (2.30)

Boundary condition one: $\bar{C}(0,t) = C_0$ (2.31)

Boundary condition two: $\frac{\partial \bar{C}}{\partial x}(L,t) = 0$ (2.32)

which imply that there is no dispersive transport at x = L, and at x = 0 the concentration is specified as constant for all times. The solution in this case can be given as,

$$\bar{C} = C_0 + e^{\frac{\bar{u}x}{2D}} \sum_i a_i \, e^{-\alpha_i t} \sin \frac{\lambda_i x}{2D} \qquad (2.33)$$

where,

$$a_i = \frac{-4C_0 D\lambda_i^{\,2}}{\left(\bar{u}^2 + \lambda_i^{\,2}\right)\left(L\lambda_i - D\sin\frac{\lambda_i L}{D}\right)} \qquad (2.34)$$

$$\alpha_i = \frac{\bar{u}^2 + \lambda_i^{\,2}}{4D} \qquad (2.35)$$

and λ_i are the roots of the equation

$$\tan \frac{\lambda_i L}{2D} = -\frac{\lambda_i}{\bar{u}} \qquad (2.36)$$

The mathematical model described, Equation (2.13), above constitutes the basis of the numerical model generated in later sections. Analytical solutions given for the simplified version of the mass transport equation can only be used in the idealized versions of field problems. Nevertheless, such solutions are useful, since they contribute to a better understanding of transport phenomena. Some of these analytical solutions are used in controlling the accuracy of the finite element model developed later in the study. User oriented computer programs to evaluate some of the analytical solutions given in this section are presented in Appendix I for completeness.

3.0 FIELD PARAMETERS

The one dimensional mass transport equation described in Section 2 involves two important parameters, namely the longitudinal diffusion coefficient and the first order decay constant, which need to be studied in detail. There have been various efforts to estimate these parameters in natural rivers for different pollutants and different flow conditions, and a considerable volume of literature has accumulated over the years. It is clear that predictions of system behavior based on mathematical simulation techniques may be misleading if the physical mechanisms involved are not accurately reflected in the model. Furthermore, even where the model does describe the mechanisms in the prototype properly, poor results may be obtained if the data available for use in the estimation of rate constants and coefficients are insufficient.

The importance of the proper description of the physical parameters involved is obvious. Thus, in this section, a summary of the more important results obtained in relation to the estimation of the longitudinal diffusion coefficient is presented in chronological order. The numerical model developed includes three predictive equations for this parameter as a default value. These equations are used in case the user does not supply the longitudinal diffusion coefficient as data for the problem being analyzed. Two of the predictive equations are chosen from the available literature as will be described further in this section and the third equation is developed in this study as an extension of one of the previous equations. The decay constant on the other hand is incorporated into the model as the half lives of several radioactive elements for case studies which involve radioactive pollution transport. If radioactive elements other than the ones discussed in this section are studied, or if decay or uptake of other related physical phenomena are to be modeled, then the decay constant of such a problem should be supplied as a part of the data. Other than these two parameters, kinematic characteristics of flow and geometric characteristics of the river reach should be given as data. As mentioned earlier, no effort is made to generate these variables at this stage.

3.1 Longitudinal Diffusion Coefficient

Longitudinal dispersion is the action by which a mass of pollutant is diluted and spread out as the flow takes place in the down stream direction. In one dimensional applications the effective diffusion coefficient representing this phenomena is a cross-sectional average value integrated over the cross-sectional area perpendicular to flow and represents the sum of two components. The first component involves the cross product of the longitudinal velocity and concentration deviations, and represents a mass transport associated with the non-uniform velocity distribution. The second component involves the spatial mean value of the Eddy diffusivity. The integral component is represented by a Fickian expression and the sum of the two diffusive effects is termed as longitudinal dispersion.

The first important study of dispersion in turbulent shear flow was published by G. I. Taylor in 1954. Since then, various equations have been used to predict this coefficient both in natural streams and in laboratory channels. A summary of such efforts are given in Table 3.1-1 in chronological order. Detailed discussions of various aspects of these predictive models can be found in Fisher (1979) and Glover (1964). In this study, the equation suggested by Fisher (Eqn. 8, Table 3.1-1) and the equation suggested by Liu (Eqn. 10, Table 3.1-1) are used as the first two predictive models

TABLE 3.1-1

SUMMARY OF EQUATIONS DEVELOPED TO ESTIMATE THE LONGITUDINAL DISPERSION COEFFICIENT

No.	Reference	Equation	Remarks
1.	Taylor (1954)	$D = 10.1\ (r\ U_*)$	For long straight circular pipes
2.	Thomas & Elder (1959)	$D = 5.9\ (d\ U_*)$	For infinitely wide open channels, obtained from analytic and experimental work
3.	Elder (1960)	$D = 22.6\ n\ \bar{u}\ d^{0.833}$	Natural streams, experimental work
4.	Patterson & Gloyna (1966)	$D = k_1 \left(\frac{\bar{u}}{\ln(\frac{b}{d})}\right)^{k_2}$	Experimental work, k_1= 0.258, k_2= 0.83 for laboratory flumes. k_1= 0.229, k_2=0.269 for natural streams
5.	Fisher (1966)	$D = 0.3\ \frac{\overline{u'^2}\ l^2}{R \sqrt{g R S_e}}$	Natural streams
6.	Gloyna (1971)	$D = 3.26\ \bar{u}^{0.607}$	Experimental work, for stream velocities ranging from 0.33 to 3.3 ft/sec.
7.	McQuivey & Keefer (1974)	$D = 0.058\ \frac{Q}{S_e b}$	Experimental data analysis
8.	Fisher (1975)	$D = 0.011\ \frac{\bar{u}^2\ b^2}{d\ \ U_*}$	An extension of Eqn. 5
9.	Bansal (1976)	$\log K \frac{\bar{u}}{v} \frac{D}{vH} = 6.45 - 0.762 \log\left(\frac{\rho v H}{\mu}\right)$ $H = A/B \qquad v = x/t_p$	For natural streams, based on Reynolds number and channel configuration
10.	Liu (1977)	$D = \beta\ \frac{Q^2}{U_* R^3}\ ,\ \beta = 0.18\ \left(\frac{U_*}{\bar{u}}\right)^{1.5}$	For natural streams, based on data analysis.

TABLE 3.1-1 (cont'd)

Description of variables used in Table I :

A : Cross-sectional area
b : Width of channel
B : Top width of flow
D   Longitudinal dispersion coefficient
d : Depth of flow
K : Regional dispersion factor
l : Characteristic length
μ : Coefficient of viscosity
n : Mannings roughness coefficient
Q : Discharge
r : Pipe radius
R : Hydraulic radius
ρ : Density
S_e: Slope of the energy grade line
$\underline{t}_p$: Time to peak arrival of concentration
$\bar{u}$: Mean velocity
U_*: Shear velocity
u': Spatial velocity variation from mean velocity
x : Reach length

for estimating the longitudinal dispersion coefficient. In addition to these two, a modified version of the equation suggested by Liu (1977) has been developed and incorporated into the computer model as a third alternative. The reason for choosing and modifying Liu's equation is twofold; first, data required to predict the longitudinal diffusion coefficient can be reduced considerably if this equation is used; second, the accuracy of this equation is considerably higher when results are compared with the results of other predictive models. The equation was modified to incorporate the effects of the sinuousity of the channel into the longitudinal diffusion coefficient.

The first alternative that can be chosen to predict the longitudinal equation is the equation given by Fisher (1975). This equation can be given as,

$$D = 0.011 \frac{\bar{u}^2 b^2}{d U_*} \tag{3.1}$$

which is an extension of the equation suggested by the same researcher in 1966. In order to use this equation to predict the longitudinal dispersion coefficient at a certain point in a river reach, the user must supply the variables $\bar{u}$, b, d and U_* as data at that specific location. Equation (3.1) is incorporated into the transport model developed in this study as a first alternative.

The second alternative equation used in the model is the equation suggested by Liu and is given as,

$$D = \beta \frac{Q^2}{R^3 U_*} \tag{3.2}$$

where β is a dimensionless coefficient for natural streams, Q is the discharge,

U_* is the shear velocity and R is the hydraulic radius of the channel. The dimensionless coefficient β is given as,

$$\beta = 0.18 \left(\frac{U_*}{\bar{u}}\right)^{1.5} \tag{3.3}$$

The form of the Equation (3.3) is arrived at based on the assumptions that most streams are sinuous or tortuous, and they contain sudden contractions and expansion, dead zones of water, islands, sand bars, bridges, etc. In general, these factors not only enhance dispersion, but also increase the resistance to flow, thus one may expect a correlation between the dimensionless coefficient, β, and the resistance coefficient, f, of the Darcy-Weisbach equation. Thus, instead of using the parameter, f, one may use the parameter, $(U_*/\bar{u})$, which is nothing other than $\sqrt{f/8}$. Deciding on the form of Equation (3.3) through these arguments, the coefficients of the same relation are arrived at by analyzing data collected from various experimental studies, and the curve fitting is done by observation. Equation (3.2) and (3.3) are also incorporated into the transport model developed in this study as a second alternative in predicting the longitudinal diffusion coefficient.

A third alternative to Equations (3.1) and (3.2) is developed in this study as an extension of the equation suggested by Liu (1977). The need for such an extension originated from the idea that sinuousity of river reaches, which plays an important role on the magnitude of the longitudinal dispersion coefficient, can be represented in a much better way if one introduces a parameter which reflects this effect better than the ratio $(U_*/\bar{u})$ chosen by Liu which mainly reflects the local resistance to flow. A second reason to develop another equation originated from the need to perform a more rigorous data analysis on an extended data base than was used by Liu in predicting the coefficients of Equation (3.3). A detailed literature survey increased the data base from (15), as was the case in Liu (1977), to (72). The form of the predictive equation is assumed as,

$$D = \alpha (\frac{U_*}{\bar{u}})^{\beta} (\frac{L_r}{L_s})^{\gamma} (\frac{Q^2}{R^3 U_*}) \qquad (3.4)$$

which has essentially the same form as Equations (3.2) and (3.3) except the ratio (L_r/L_s) which is the ratio of the actual length of the river at the specific site considered divided by the length of the straight line joining the two ends of the river reach for the same site. This ratio is chosen to reflect the sinuosity of the river reach as a first approximation although other more rigorous descriptions have been used in the literature earlier. A least squares curve fitting technique is used in arriving at the values of the coefficients α, β and γ in comparison to the curve fitting by observation used by Liu. The resulting equation has the form seen below,

$$D = (0.0019) (\frac{U_*}{\bar{u}})^{0.25} (\frac{L_r}{L_s})^{4.56} (\frac{Q^2}{R^3 U_*}) \qquad (3.5)$$

The data used in this curve fitting process is summarized in Table 3.1-2 below. In Table 3.1-3 a comparison of some of the longitudinal diffusion coefficients predicted by these three equations are given. Results indicate that all three equations have similar reliabilities given the state of art of predicting longitudinal coefficient using limited data. However, since Equation (3.5) is derived using a least squares technique, the longitudinal dispersion coefficients predicted using this equation and the data presented in Table 3.1-2 results in much lower deviations from the observed values in comparison to similar predictions done using Equations (3.1) and (3.2)

TABLE 3.1-2

NATURAL RIVER AND LABORATORY FLUME DATA

OBSERVED LONGITUDINAL DISPERSION COEFFICIENTS

Data Number	Width (m)	Depth (m)	$\bar{u}$ (m/s)	U_* (m/s)	R (m)	Q (m^3/s)	L_r/L_s	D (m^2/s)	Location Description	Ref. No.
1	15.70	N/D	0.235	0.0790	0.491	1.54	1.83	15.00	Copper Cr. Gate City VA.	1
2	67.4	N/D	0.252	0.0580	0.953	9.14	1.07	9.10	Clinch River, Speers Ferry VA.	1
3	17.1	N/D	0.187	0.1040	0.378	0.99	1.83	9.10	Copper Cr. Gate City VA.	1
4	34.4	N/D	0.164	0.0520	0.851	3.96	2.46	26.80	Powell River, Sneedville, TN.	1
5	34.7	N/D	0.181	0.0460	0.666	6.80	1.27	19.70	Clinch River, Clinchport, VA.	1
6	18.2	N/D	0.616	0.1040	0.848	8.49	1.83	41.80	Copper Cr. Gate City, VA.	1
7	60.0	N/D	0.838	0.0850	1.840	84.90	1.07	11.10	Clinch River, Speers Ferry, VA.	1
8	24.7	N/D	0.638	0.0430	1.560	25.50	1.00	17.70	Coachella Canal, Calif.	1
9	24.7	N/D	0.713	0.0430	1.560	26.90	1.00	17.70	Coachella Canal, Calif.	1
10	59.1	N/D	0.658	0.0760	1.470	51.00	1.07	11.10	Clinch River, Speers Ferry VA.	1
11	16.1	N/D	0.241	0.0760	0.454	1.36	1.83	15.40	Copper Cr. Gate City VA.	1
12	187.8	N/D	1.710	0.0770	3.050	957.00	1.39	1490.00	Missouri River, Blair,Omaha,NEB.	1
13	29.9	N/D	0.320	0.0490	1.100	8.78	1.57	6.50	Green-Duwamish River, Seattle WA	1
14	48.8	N/D	0.271	0.0560	6.330	107.1	1.00	3.56	Chicago Canal	1
15	48.8	N/D	0.271	0.0190	6.330	107.1	1.00	3.61	Chicago Canal	1
16	N/D	0.306	0.454	0.0190	0.108	0.043	1.00	0.051	Flume-Triangular	2
17	N/D	0.449	0.701	0.0275	0.159	0.1414	1.00	0.081	Flume-Triangular	2
18	N/D	0.607	0.787	0.0293	0.215	0.2895	1.00	0.122	Flume-Triangular	2
19	2.42	0.145	0.687	0.0305	0.123	0.2266	1.00	0.075	Flume-Rectangular	2
20	2.42	0.166	0.423	0.0183	0.146	0.1700	1.00	0.065	Flume-Rectangular	2
21	2.42	0.150	0.156	0.0171	0.134	0.0567	1.00	0.043	Flume-Rectangular	2
22	2.42	0.150	0.624	0.0857	0.134	0.2266	1.00	0.119	Flume-Rectangular	2
23	1.22	0.300	0.163	0.0066	0.201	0.0581	1.00	0.039	Flume-Rectangular	2
24	0.33	0.510	0.632	0.0270	0.170	0.1643	1.00	0.081	Flume-Rectangular	2
25	0.042	0.116	0.376	0.0428	0.0175	0.0018	1.00	0.0355	Flume #100 Rectangular	3
26	0.041	0.052	0.194	0.0394	0.0148	0.00042	1.00	0.0106	Flume #200 Rectangular	3
27	1.10	0.166	0.362	0.0366	0.1270	0.0661	1.00	0.0456	Flume #300 Rectangular	3
28	1.10	0.229	0.489	0.0454	0.1617	0.1230	1.00	0.0742	Flume #400 Rectangular	3
29	0.851	0.046	0.323	0.0151	0.0415	0.0126	1.00	0.0072	Flume #1200 Rectangular	3
30	0.851	0.091	0.299	0.0129	0.0750	0.0232	1.00	0.0169	Flume #1300 Rectangular	3
31	0.851	0.137	0.262	0.0112	0.1036	0.0305	1.00	0.0191	Flume #1400 Rectangular	3
32	0.851	0.065	0.194	0.0103	0.0564	0.0107	1.00	0.0074	Flume #1500 Rectangular	3

TABLE 3.1-2 (continued)

Data Number	Width (m)	Depth (m)	$\bar{u}$ (m/s)	U_* (m/s)	R (m)	Q (m^3/s)	L_r/L_s	D (m^2/s)	Location Description	Ref. No.
33	0.851	0.064	0.220	0.0140	0.0556	0.012	1.00	0.0231	Flume #1600 Rectangular	3
34	1.10	0.139	0.242	0.0265	0.1110	0.037	1.00	0.0578	Flume #2300 Rectangular	3
35	1.10	0.094	0.212	0.0308	0.0803	0.0218	1.00	0.0427	Flume #2400 Rectangular	3
36	1.10	0.184	0.222	0.0259	0.1379	0.0449	1.00	0.0626	Flume #2500 Rectangular	3
37	1.10	0.069	0.269	0.0136	0.0613	0.0204	1.00	0.0177	Flume #2600 Rectangular	3
38	1.10	0.128	0.362	0.0162	0.1038	0.0510	1.00	0.0236	Flume #2700 Rectangular	3
39	0.381	0.035	0.251	0.0202	0.0303	0.0036	1.00	0.222	Flume #2800 Trapezoidal, z=1	3
40	0.381	0.047	0.454	0.0359	0.0391	0.00913	1.00	0.317	Flume #2900 Trapezoidal, z=1	3
41	0.381	0.035	0.451	0.0351	0.0303	0.00657	1.00	0.559	Flume #3000 Trapezoidal, Z=1	3
42	0.3175	0.035	0.444	0.0348	0.0296	0.00548	1.00	0.408	Flume #3100 Trapezoidal, z=1	3
43	0.3175	0.021	0.453	0.0328	0.0189	0.00322	1.00	0.565	Flume #3200 Trapezoidal, z=1	3
44	0.3175	0.034	0.483	0.0249	0.0289	0.00577	1.00	0.0282	Flume #3300 Trapezoidal, z=1	3
45	0.1905	0.021	0.461	0.0388	0.0178	0.00205	1.00	0.254	Flume #3400 Trapezoidal, z=1	3
46	48.8	8.07	0.270	0.0191	8.07	106.330	1.00	3.00	Chicago Ship Canal	4
47	200.00	2.70	1.550	0.0740	2.70	837.000	1.34	1500.00	Missouri River, Siou City, NEB	5
48	16.00	0.49	0.270	0.0800	0.49	2.12	1.83	2.00	Copper Cr. Gate City, VA.	6
49	18.00	0.85	0.600	0.1000	0.85	9.18	1.83	21.00	Copper Cr. Gate City, VA.	6
50	16.00	0.49	0.260	0.0800	0.49	2.04	1.83	9.50	Copper Cr. Gate City, VA.	6
51	47.00	0.85	0.320	0.0670	0.85	12.78	1.45	14.00	Clinch River, TN.	6
52	60.00	2.10	0.940	0.1040	2.10	118.44	1.45	54.00	Clinch River TN.	6
53	53.00	2.10	0.830	0.1070	2.10	92.38	1.45	47.00	Clinch River TN.	6
54	19.99	0.40	0.160	0.1160	0.40	1.22	1.83	9.90	Copper Cr. Gate City VA.	6
55	34.00	0.85	0.150	0.0550	0.85	4.34	2.46	9.50	Powell River, Sneedville, TN.	6
56	36.00	0.58	0.210	0.0490	0.58	4.38	1.27	8.10	Clinch River, Clichport VA.	6
57	24.00	1.56	0.710	0.0430	1.56	26.58	1.00	9.60	Coachella Canal Calif.	7
58	26.00	0.94	0.340	0.0670	0.94	8.31	1.66	33.00	Bayou Anacoco, LA.	7
59	37.00	0.91	0.400	0.0670	0.91	13.47	1.66	39.00	Bayou Anacoco, LA.	7
60	64.00	0.76	0.670	0.2700	0.76	32.59	1.33	35.00	Nooksack River, WASH.	7
61	59.00	1.10	0.880	0.1200	1.10	57.11	1.08	42.00	Bighorn River, MONT.	7
62	69.00	2.16	1.550	0.1700	2.16	231.01	1.08	160.00	Bighorn River, MONT.	7
63	25.00	0.58	1.010	0.1400	0.58	14.65	1.78	14.00	John Day River, Oregon	7
64	34.00	2.47	0.820	0.1800	2.47	68.86	1.78	65.00	John Day River, Oregon	7
65	16.00	0.43	0.370	0.0500	0.43	2.55	1.49	14.00	Comite River, LA.	7
66	104.00	2.04	0.580	0.0500	2.04	123.05	1.80	315.00	Sabine River, LA.	7
67	127.00	4.75	0.640	0.0800	4.75	386.08	1.80	670.00	Sabine River, LA.	7
68	70.00	2.35	0.430	0.1000	2.35	70.74	1.64	110.00	Yadkin River, LA.	7
69	72.00	3.84	0.760	0.1300	3.84	210.12	1.64	260.00	Yadkin River, NC.	7
70	N/D	3.45	0.680	0.3450	1.73	17.75	1.00	0.76	Canal - Trapezoidal	8

TABLE 3.1-2 (cont'd)

DETERMINATION OF SINUOSITY(L_R/L_S) RATIO

NAME OF STREAM	USGS QUAD SHEET NAME	SCALE	L_R(inches)	L_S(inches)	L_R/L_S
Copper Creek	Gate City, Virginia $7\frac{1}{2}$ minute	1:24K	38.0	20.8	1.83
Powell River	Back Valley, Tenn. (West of Sneedville, TN) $7\frac{1}{2}$ minute	1:24K	52.0	21.1	2.46
Duwamish-Green River	Des Moines, Washington $7\frac{1}{2}$ minute	1:24K	30.1	19.2	1.57
John Day River (Middle Fork)	Ritter, Oregon 15 minute	1:62.5K	24.5	13.8	1.78
Sabine River	Haddens, Louisiana-Tex. $7\frac{1}{2}$ minute	1:24K	47.0	26.1	1.80
Bayou Anacoco	Newllano, Louisiana $7\frac{1}{2}$ minute	1:24K	11.6	7.0	1.66
Nooksack River (North Fork)	Maple Falls, Washington $7\frac{1}{2}$ minute	1:24K	20.1	15.1	1.33
Yadkin River	Copeland, North Car. $7\frac{1}{2}$ minute	1:24K	31.0	18.9	1.64
Comite River	Comite, Louisiana $7\frac{1}{2}$ minute	1:24K	37.0	24.9	1.49
Big Horn River	Lemonade Springs, Mont. $7\frac{1}{2}$ minute	1:24K	19.0	17.6	1.08
Clinch River	Looney's Gap, Tennessee $7\frac{1}{2}$ minute	1:24K	27.6	19.0	1.45
Clinch River (Clinchport, VA)	Clinchport, Virginia $7\frac{1}{2}$ minute	1:24K	26.5	20.9	1.27

TABLE 3.1-2 (cont'd)

DETERMINATION OF SINUOSITY(L_R/L_S) RATIO

NAME OF STREAM	USGS QUAD SHEET NAME	SCALE	L_R(inches)	L_S(inches)	L_R/L_S
Clinch River (Speers Ferry, VA)	Clinchport, Virginia 7½ minute	1:24K	26.5	20.9	1.27
Missouri River (Blair to Plattsmouth, Nebraska)	Modale, Iowa-Neb Loveland, Iowa-Neb Council Bluff North, Iowa-Neb Omaha North, Neb.-Iowa Council Bluff South, Iowa-Neb. Omaha South, Neb.-Iowa Pacific Junction, Iowa-Neb. Plattsmouth, Neb.-Iowa (All 7½ minute)	1:24K (ALL)	160.1	115.3	1.39
Missouri River (Sioux City, Iowa to Blair, Nebraska)	Sioux City South, Neb-S.Dak Salix, Iowa-Neb Homer, Neb.-Iowa Albaton, Iowa-Neb. Tekamah NW, Neb.-Iowa Little Sioux, Iowa-Neb. Mondamin, Iowa-Neb. Modale, Iowa-Neb. Loveland, Iowa-Neb. Council Bluff North, Iowa-Neb. Omaha North, Neb.-Iowa Council Bluff South, Iowa-Neb. Omaha South, Neb.-Iowa Pacific Junction, Iowa-Neb. Plattsmouth, Neb.-Iowa (All 7½ minute)	1:24K (ALL)	347.7	260.0	1.34

TABLE 3.1-2 (cont'd)

NOTES

I. N/D: No data available in reference for this item.

II . REFERENCES

Reference Number	Author(s)
1	Liu, H.; 1977
2	Glover, R.; 1964
3	Fischer; 1967
4	Thomas; 1958
5	Yotsukura; 1970
6	Godfrey & Fredrick; 1970
7	McQuivey & Keefer; 1974
8	Schuster; 1965

TABLE 3.1-3

VERIFICATION OF LONGITUDINAL DISPERSION PREDICTION EQUATIONS

Reference	Observed (m^2/s)	Eq. 3.1 (m^2/s)	Eq. 3.2 (m^2/s)	Eq. 3.5 (m^2/s)
Owens, Edwards and Gibbs	4.6	2.17	12.11	1.95
Miller and Richardson				
Test #1	0.052	0.095	0.140	0.027
Test #2	0.266	0.166	0.244	0.047
Test #4	0.067	0.056	0.188	0.020
Test #7	0.147	0.046	0.197	0.025
Test #8	1.080	0.076	0.364	0.026
Test #9	6.127	0.110	0.518	0.039

Note: Miller, A. C., and Richardson, E. V., (1974). "Diffusion and Dispersion in Open Channel Flow", Proc. A.S.C.E., Jr. Hyd. Div., 100, 159-171.
Owens, M., Edwards, R. W. and Gibbs, J. W., (1964). "Some Reaeration Studies in Streams", Air Water Pollut. Int. Jr., 8, 469-486.

Thus, the choice between these three equations should be made by the user depending on the availability of data. As stated earlier, all three equations are incorporated into the computer model developed in this study.

3.2 Decay Coefficient

In the case of radioactive spills the rate of decay of the radioactive material is an important aspect of the study especially for radionuclides with high rates of decay. The computer model generated in this study contains the half-lives of sixty-three radionuclides from which the decay constants can be generated. For any pure radioactive substance, the rate of decay is usually described by its half life Λ, i.e, the time it takes for a specified source material to decay to half its initial activity. Given this definition, the decay constant, K (sec^{-1}), can be given as,

$$K = \frac{Ln2}{\Lambda} \qquad (3.6)$$

For a case study involving one of the radionuclides the user need only to supply the number of nuclide given in the list below and the time unit chosen in the study. The model automatically incorporates the decay constant into the model. Details of data preparation for this phase is given in Section 5 of this report. List of radionuclides and associated half lives given in the table below is obtained from R. S. Booth (1975).

TABLE 3.2-1

RADIONUCLIDES AND RADIOACTIVE HALF-LIFE

No:	Radionuclide	Half-life	No:	Radionuclide	Half-life
1.	H-3	12.3 y	2.	C-14	5730 y
3.	Na-22	2.58 y	4.	Na-24	15.0 h
5.	P-32	14.3 d	6.	S-35	88 d
7.	Sc-46	84 d	8.	Cr-51	27.7 d
9.	Mn-54	313 d	10.	Fe-55	2.7 y
11.	Fe-59	45 d	12.	Co-57	276 d
13.	Co-58	71 d	14.	Co-60	5.26 y
15.	Ni-63	92 y	16.	Cu-64	12.8 h
17.	Zn-65	244 d	18.	Zn-69m	14 h
19.	Rb-86	18.7 d	20.	Sr-89	50.5 d
21.	Sr-90	28.5 y	22.	Y-90	64.2 h
23.	Sr-91	9.7 h	24.	Y-91	59 d
25.	Y-93	10 h	26.	Zr-95	63 d
27.	Nb-95	35 d	28.	Zr-97	17 h
29.	Mo-99	66 h	30.	Ru-103	41 d
31.	Rh-105	35.5 h	32.	Ru-106	1.0 y
33.	Ag-110m	270 d	34.	Sb-122	2.8 d
35.	Sb-124	60.2 d	36.	Sn-125	9.5 d
37.	Sb-125	2.7 y	38.	Te-125m	58 d
39.	Sb-127	93 h	40.	Te-127m	109 d
41.	Te-127	9.3 h	42.	Te-129m	33 d
43.	I-130	12.6 h	44.	Te-131m	30 h
45.	I-131	8.05 d	46.	Te-132	77 h
47.	I-133	20.9 h	48.	Cs-134	2.1 y
49.	I-135	6.7 h	50.	Cs-136	13 d
51.	Cs-137	30.0 y	52.	Ba-140	12.8 d
53.	La-140	40.2 h	54.	Ce-141	32 d
55.	Ce-143	32 h	56.	Pr-143	13.7 d
57.	Ce-144	290 d	58.	Nd-147	11.3 d
59.	Pm-147	2.6 y	60.	Ta-182	115 d
61.	W-185	74 d	62.	W-187	24 h
63.	Np-239	2.3 d			

Note : y : Years
d : Days
h : Hours

4.0 NUMERICAL MODEL

A one dimensional finite element model is used to approximate the mathematical model developed in the previous sections. The first step in such a discretization process is the division of the solution region into a finite number of subregions which are called elements. This process is dictated by the need to find an alternative form of the equilibrium equations which will be easier to solve than the governing equations of the continuum. The modified conceptualization of the system results in a set of simultaneous algebraic equations rather than differential equations, thus simplifying the solution considerably. The size and distribution of the elements and the approximation used in each element are arbitrary. Given the one dimensional nature of the problem analyzed, two nodal one dimensional linear elements are used in the solution process in this study. A summary of the steps involved in generating finite element matrix equations for the mathematical model studied is given below. A detailed description of finite element programming is given by Zienkiewicz (1971) and Desai (1972).

A finite element approximation to Equation (2.13) can be obtained through a Galerkin approach. Over an element the residual, R, for Equation (2.13) can be given as,

$$R(\bar{C}) = \frac{\partial \bar{C}}{\partial t} + \bar{u}\frac{\partial \bar{C}}{\partial x} - \frac{1}{A}\frac{\partial}{\partial x}\left\{AD\,\frac{\partial \bar{C}}{\partial x}\right\} + K\bar{C} \qquad (4.1)$$

Weighing the residual with respect to a weighing function N_m yields,

$$I^e = \int_{\ell^e} N_m\left\{\left\{\frac{\partial}{\partial t} + \bar{u}\frac{\partial}{\partial x} - \frac{1}{A}\frac{\partial}{\partial x}\left\{AD\frac{\partial}{\partial x}\right\} + K\right\}N_k\bar{C}_k\right\}d\ell^e \quad m,k = 1,...,n \qquad (4.2)$$

where repeated indices indicate summation, n is the number of nodes, N_m is the weighing function which is chosen as the finite element shape functions in a Galerkin formulation and $\bar{C}_k$ is the nodal value of the dependent variable in an element. Equation (4.2) is written for a single element; however, it is understood that the same procedure is applied to the entire medium. The interpolation used to approximate $\bar{C}$ over an element can be given as,

$$\bar{C} = N_k \bar{C}_k \qquad k = 1,\ldots,n \tag{4.3}$$

where $\bar{C}_k$ are the unknown nodal values of the dependent variable as described above and N_k is the interpolating polynomial used to approximate, $\bar{C}$, in an element. For a typical two nodal element these polynomials are given as,

$$\left.\begin{aligned} N_1(\xi_1,\xi_2) &= \xi_1 \\ N_2(\xi_1,\xi_2) &= \xi_2 \end{aligned}\right\} \tag{4.4}$$

where ξ_1, and ξ_2 are natural coordinate systems for a two nodal element defined as,

$$\xi_1 = \frac{\ell - x}{\ell}\,, \quad \xi_2 = \frac{x}{\ell} \tag{4.5}$$

where (x) is the local coordinate.

Equation (4.2) can be expanded as,

$$I^e = \int_{\ell^e} N_m N_k \frac{\partial \bar{C}_k}{\partial t} d\ell^e + \int_{\ell^e} N_m \left\{\bar{u}\frac{\partial N_k}{\partial x}\right\}\bar{C}_k d\ell^e + \int_{\ell^e} K N_m N_k \bar{C}_k d\ell^e + \int_{\ell^e} \frac{N_m}{A}\frac{\partial}{\partial x}\left\{AD\frac{N_k}{x}\right\}\bar{C}_k d\ell^e$$

$$m,k = 1,\ldots,n. \tag{4.6}$$

Assuming (A) and (D) to be constant in an element, one can integrate the last term by parts yielding,

$$\int_{\ell^e} N_m\left[\frac{1}{A}\frac{\partial}{\partial x}\left\{AD\frac{\partial N_k}{\partial x}\right\}C_k\right] d\ell^e = DN_m\frac{\partial \bar{C}}{\partial n}\bigg|_B - \int_{\ell^e} D\frac{\partial N_m}{\partial x}\,\frac{\partial N_k}{\partial x}\bar{C}_k d\ell^e \tag{4.7}$$

The first term on the right-hand side in Equation (4.7) describes the

Neuman type boundary conditions and can be specified as a known value of the normal derivative $\frac{\partial \bar{C}}{\partial n}$. Thus, the term $(D\frac{\partial \bar{C}}{\partial n}\Big|_B)$ describes the known flux on the boundaries. Substitution of Equation (4.7) into Equation (4.6) and minimizing the residual leads to element equations in matrix form as,

$$[P^e]\{\frac{\partial \bar{C}}{\partial t}\} + [S^e]\{\bar{C}\} = \{F^e\} \qquad (4.8)$$

where $\{\frac{\partial \bar{C}}{\partial t}\}$ and $\{\bar{C}\}$ are vectors of nodal time derivatives and nodal values of the dependent variable and $[P^e]$, $[S^e]$ are the local mass and stiffness matrices defined as,

$$[P^e] = \int_\ell N_m N_k d\ell^e \qquad m, k = 1,\ldots,n. \qquad (4.9)$$

$$[S^e] = \int_\ell [\bar{u}N_m\frac{\partial N_k}{\partial x} + D\frac{\partial N_m}{\partial x}\frac{\partial N_k}{\partial x} + KN_mN_k]d\ell^e \qquad m, k = 1,\ldots,n. \qquad (4.10)$$

and $\{F^e\}$ is the local load vector defined by the boundary terms of Equation (4.7). An evaluation of these matrices for a typical two nodal element of length (ℓ) with the assumption of D, K and $\bar{u}$ being constant in an element yields

$$[P^e] = \frac{\ell}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \qquad (4.11)$$

$$[S^e] = \begin{bmatrix} (\frac{D}{\ell} - \frac{\bar{u}}{2} + \frac{K\ell}{3}) & (\frac{-D}{\ell} + \frac{\bar{u}}{2} + \frac{K\ell}{6}) \\ (\frac{-D}{\ell} - \frac{\bar{u}}{2} + \frac{K\ell}{6}) & (\frac{D}{\ell} + \frac{\bar{u}}{2} + \frac{K\ell}{3}) \end{bmatrix} \qquad (4.12)$$

Following formation of $[P^e]$, $[S^e]$ and $\{F^e\}$ a routine finite element assembly process yields for the global system a similar equation which can be given as,

$$[P]\ \{\frac{\partial \bar{C}}{\partial t}\} + [S]\ \{\bar{C}\} = \{F\} \qquad (4.13)$$

Thus, the partial differential Equation (2.13) is reduced to a finite element matrix equation system through a finite element Galerkin process. An implicit time integration scheme can now be used to integrate Equation (4.13) step by step, Wilson (1962). This process leads to the matrix system,

$$(\frac{2}{\Delta t}[P] + [S])\ \{\bar{C}\}_{t+\Delta t} = (\frac{2}{\Delta t}[P] - [S])\ \{\bar{C}\}_t + 2\{F\} \qquad (4.14)$$

Thus, the problem at this stage is reduced to the solution of a simultaneous algebraic system for the unknown nodal values of, $\bar{C}_k$, at time $(t + \Delta t)$ starting from an initial condition on $\bar{C}$. Repeating the same process with increments of, Δt, yields a solution for, $\bar{C}$, in time and space coordinates.

The finite element model generated above is coded in Fortran IV computer language. The complete listing of "Transport Model I" (TRMOD I) is given in the Appendix II. Several user oriented data generation routines are added to TRMOD I in order to simplify the data preparation process for the user. Although the model basically uses the finite element computation process described above, several other variations of possible finite element approximations in an element are also incorporated into the model. For example, in the derivation given above D, $\bar{u}$ and K are assumed to be constant in each element. In finite element approximations, these variables can also be described at the nodes and their variation in an element can be described in terms of an interpolating polynomial. Although the derivation of such specific cases will not be given here, the resulting matrices have been computed and the "TRMOD I" model is coded in such a way to let the user choose the specific approximation desired for a given problem. Typically, if D, $\bar{u}$ and K are assumed to vary linearly in an element, Equation (4.12) will take the form,

$$[S^e] = \begin{bmatrix} \left(\frac{D_1}{2\ell}+\frac{D_2}{2\ell}-\frac{\bar{u}_1}{3}-\frac{\bar{u}_2}{6}+\frac{K_1\ell}{4}+\frac{K_2\ell}{12}\right) & \left(-\frac{D_1}{2\ell}-\frac{D_2}{2\ell}+\frac{u_1}{3}+\frac{u_2}{6}+\frac{K_1\ell}{12}+\frac{K_2\ell}{12}\right) \\ \left(-\frac{D_1}{2\ell}-\frac{D_2}{2\ell}-\frac{\bar{u}_1}{6}+\frac{\bar{u}_2}{3}+\frac{K_1\ell}{12}+\frac{K_2\ell}{12}\right) & \left(\frac{D_1}{2\ell}+\frac{D_2}{2\ell}+\frac{u_1}{6}+\frac{u_2}{3}+\frac{K_1\ell}{12}+\frac{K_2\ell}{4}\right) \end{bmatrix} \tag{4.15}$$

which reduces back to Equation (4.12) if the nodal values of the parameters D, $\bar{u}$ and K are the same. In Equation (4.15) subscripts (1) and (2) refer to nodes one and two and a linear variation of each parameter is assumed in a typical element for each parameter. Thus, with this extension a user may choose to assume parameter D, $\bar{u}$ and K constant in an element or may choose to vary them linearly in an element. Also, control variables are included such that one may keep one parameter constant in an element while varying the others linearly in the same element. Details of the possible usable permutations are explained in Section 5. Such alternative forms may improve the accuracy of the numerical solution in regions where rapid functions in the values of the parameters D, $\bar{u}$ and K are expected.

5.0 THE COMPUTER CODE

In earlier sections of this report, an outline of the mathematical model and the finite element Galerkin formulation process used to approximate the governing partial differential equations are given. In this section, the main consideration will be the computer code generated and the description of input-output statements necessary to implement the computer code.

The "TRMOD I" computer program presented in Appendix II is written in Fortran IV computer language. The program is divided into fifteen subprograms and a main program. To avoid making the present code too complicated, some limiting features are built into it. These include the restriction to one dimensional two nodal linear elements, the restriction of the linear variation of the time derivative between time steps, and the restriction of the coefficients which are either assumed to be constant within each element or may be varied linearly throughout the element. To increase the efficiency of the code, several data generation routines are added to the program which may be utilized by the user if desired. Several default parameter generation subroutines are also added to the code in order to aid the user in cases where field parameter data is lacking. At this stage of the study, no attempt is made to generate the kinematic variables of the flow. As it stands, the "TRMOD I" computer code is capable of analyzing the time dependent one dimensional mass transport equation with the following alternative initial and boundary conditions.

Initial Conditions: Initial distribution of the concentration can be given as a constant or as a function of space coordinate. One should note here that the Dirichlet boundary conditions chosen at the end points of the solution domain should always agree with the initial condition described at those points at the initial time.

Boundary Conditions: Neuman, Dirichlet or Mixed type boundary conditions can be specified at the end points of the solution domain. Also, if desired, these boundary conditions can be changed once during the solution process specifying a time duration for the initial boundary condition. This alternative is included in order to model the timed release of pollutants in an open water environment.

5.1 Description of the Program

Various parts of the program and their specific functions are described below.

The "MAIN" Program: The Main Program controls the flow of operations in the program and performs the time space computations. Input-output subroutines, matrix generation subroutines, assembly subroutine, parameter generation subroutines and matrix solution subroutines are directly controlled from the main program.

Subroutine "ASSEM": Performs the assembly of the element matrices forming global stiffness and mass matrices. With this information, control goes back to the "MAIN" program.

Subroutine "BOUND": This subroutine introduces the Dirichlet, Neuman or Mixed boundary conditions into the final global matrices.

Subroutine "MASS": This subroutine forms the mass matrices for each element which are then assembled by the ASSEM subroutine to form the global matrices.

Subroutine "INP": All the input data for the problem to be analyzed is either generated or read in in this subroutine. More specifically, nodal pattern, element pattern, element constants, time constants, initial condition, boundary conditions are either read in or generated and printed out in here. Also, this subroutine controls the default parameter generation subroutines "DIFF" and "GAMGEN" if the user wants to generate a diffusion coefficient and/or a decay constant for a specific point or a region in the solution domain.

Subroutine "OUT": Printout of the results obtained for the problem analyzed is organized in this subroutine.

Subroutine "REDUCE": This subroutine performs the first step reduction in a Gausian Elimination solution process on a non-symmetric banded matrix, stored as a rectangular array. The control is then directed to the subroutine "SOLVE" by the "MAIN" program for the backsubstitution process.

Subroutine "SOLVE": This subroutine completes the backsubstitution process on the reduced matrices obtained from subroutine "REDUCE". The results are stored as a vector and control goes back to the "MAIN" program.

Subroutine "MLTPLY": Performs the multiplication of a non-symmetric banded matrix, stored as a rectangular array, with a vector. The resultant vector is stored in a separate location, and the control goes back to the "MAIN" program.

Subroutine "GAMGEN": This subroutine generates the half lives of sixty-two radioactive elements if the problem is designed to analyze transport characteristics of the elements given in Section

Subroutine "DIFF": This subroutine generates the longitudinal diffusion coefficient at a given location in the solution region. As described in Section 3, user may choose to use three alternative generation equations for this purpose. Namely, equations given by Fisher (1975), Liu (1977) and the equation generated in this report can be used to predict the diffusion coefficient as a default valve.

Subroutines "EL1N1", "EL2N2", "EL2N3", "EL2N4", and "EL2N5": These subroutines form the stiffness matrices for each element which is then assembled by the subroutine "ASSEM" to form the global matrices. Element matrices generated with these subroutines differ from one another with regard to the assumptions made in describing the constants of the problem. Specifically, the following alternatives are considered in each subroutine.

Subroutine "EL2N1": Parameters D, $\bar{u}$ and K are assumed to be constant in each element.

Subroutine "EL2N2": Parameters D, $\bar{u}$ and K are assumed to vary linearly in each element.

Subroutine "EL2N3": Parameters D and K are assumed to be constant in each element and $\bar{u}$ is assumed to vary linearly in the same element.

Subroutine "EL2N4": Parameters $\bar{u}$ and K are assumed to vary linearly in each element and D is assumed to be constant in the same element.

Subroutine "EL2N5": Parameters D and $\bar{u}$ are assumed to vary linearly in each element and K is assumed to be constant in the same element.

5.2 Control Cards and Input Data

The first step in the analysis is to select a finite element representation for the region of interest. Elements and nodal points are then numbered in two numerical sequences, each starting with one. The following group of punched cards are necessary to operate the program.

5.2.1 CONTROL CARD I: (6I2)

Column 2	(1) Indicates the use of subroutine "EL2N1" (2) Indicates the use of subroutine "EL2N2" (3) Indicates the use of subroutine "EL2N3" (4) Indicates the use of subroutine "EL2N4" (5) Indicates the use of subroutine "EL2N5"
Column 4	(0) Indicates a time independent problem (1) Indicates a time dependent problem
Column 6	Number of Neuman boundary conditions
Column 8	Number of Dirichlet boundary conditions
Column 10	Number of Mixed boundary conditions
Column 11	(0) Indicates that decay constant will not be generated (1) Indicates the generation of the decay constant using subroutine "GAMGEN"

5.2.2 IDENTIFICATION CARD: (20A4)

Columns 1 to 80 of this card contain information to be printed as the title.

5.2.3 CONTROL CARD II: (2I5)

Columns 1-5	Number of reference nodal points. Data between these reference nodes will be generated assuming equal spacing between elements. Also, the nodal numbering will be generated for the interior nodes from the two reference node numbers given.
Columns 6-10	Number of reference elements. Element data will be generated from the reference elements specified here.

5.2.4 CARD SET I: (I10, F10.4, I10)

In this data set, the number of data cards should be equal to the number of reference nodal points specified in Control Card II (Section 5.2.3), columns 1-5.

Columns 1-10	Node Number
11-20	x - Coordinate
21-30	(0) Indicates node generation is not requested after this node (1) Indicates node generation is requested between this node and the next one.

5.2.5 CARD SET II: (I5, 3F10.4, I5, F10.4)

In this data set, the number of data cards should be equal to the number of reference elements specified in Control Card II (Section 5.2.3), columns 6-10.

Columns 1-5	Number of elements for which data generation is requested after the reference element. Data for the following elements will be generated using the reference element data as the base data.
6-10	Constant $\bar{u}$
11-20	Constant K
21-30	Load function (a value of zero should be specified for "TRMODI" version)
31-35	(0) Indicates diffusion coefficient will be read in (>0) Indicates diffusion coefficient will be generated by one of three methods (see 3.2.6)
36-45	Constant D. (If one (1) is punched in columns 31-35 of this card, ignore the data for diffusion coefficient since this information will be generated).

5.2.6 DIFFUSION COEFFICIENT GENERATION: (4F10.3)

A diffusion coefficient data generation card should immediately follow each reference element card in the Card Set II if a value greater than zero is specified in columns 31-35.

5.2.6.1 Fisher's Equation

If in columns 31-35 of reference element card a value of one is punched, read in the following data to generate the diffusion coefficient. This prediction is based on Fisher's equation.

Columns 1-10	Width of the channel
11-20	Depth of flow
21-30	Shear velocity

5.2.6.2 Liu's Equation

If in columns 31-35 of reference element card a value of two is punched, read in the following to generate the diffusion coefficient. This prediction is based on Liu's equation.

Columns 1-10	Discharge
11-20	Hydraulic radius
21-30	Shear velocity

5.2.6.3 Derived Equation

If in columns 31-35 of reference element card a value of three is punched, read in the following data to generate the diffusion coefficient. This prediction is based on the equation derived in this report.

Columns 1-10	Discharge
11-20	Hydraulic radius
21-30	Shear velocity
31-40	Length ratio to reflect sinuousity of the channel

5.2.7 TIME DEPENDENT CONTROL CARD III: (4F10.0, I10)

If in Control Card I, the fourth column is punched as (0), then time

Time Dependent Control Cards III and the Time Dependent Data Set (Section 5.2.8) should be omitted.

Columns 1-10	Initial time
11-20	Final time
21-30	Time step
31-40	Duration of concentration spill
41-50	Printout interval

5.2.8 TIME DEPENDENT DATA SET: (I10, F10,0)

Columns 1-10	Number of nodes to be generated after this node
11-20	Initial condition at each node

5.2.9 DATA CARD FOR DECAY CONSTANT GENERATION: (2I5)

If in Control Card I, the twelfth column is punched as (0) then this data card preparation should be ignored. Otherwise, a material number obtained from Table 3. , Section 3.1, should be specified with the time units chosen to analyze the program as follows.

Columns 1-5	Material number
6-10	(1) Indicates a time unit of seconds (2) Indicates a time unit of minutes (3) Indicates a time unit of hours (4) Indicates a time unit of days

5.2.10 NEUMAN BOUNDARY CONDITION CARDS: (I10, F10.0)

If Neuman boundary conditions do not exist, then this set of cards should be omitted.

Columns 1-10	Neuman node number
11-20	Boundary condition

5.2.11 DIRICHLET BOUNDARY CONDITION CARDS: (I10, f10.0)

If Dirichlet boundary conditions do not exist, then this set of cards should be omitted.

Columns 1-10	Dirichlet node number
11-20	Boundary condition

5.2.12 MIXED BOUNDARY CONDITION CARDS: (I10, F10.0)

If mixed boundary conditions do not exist, then this set of cards should be omitted.

Columns 1-10	Mixed boundary condition node number
11-20	Boundary condition

6.0 NUMERICAL EXAMPLES

In this section a summary of numerical examples analyzed using the "TRMOD I" computer codes is presented. These examples can be classified into two groups for presentation. In the first group of examples the convective diffusion equation is studied in a nondimensional form. In this group, a set of hypothetical problems are described by varying the coefficients of the partial differential equation studied. Boundary conditions and initial conditions for these examples are specifically chosen to match the problem described in Section (2.2.E) of this report. In this way it was possible to compare the results obtained from the numerical solution with the results of the analytical solution. The analytical solution for these problems is generated using the code given in Appendix I. In the second group of examples, some numerical studies which predict mass transport in natural river are considered. This phase constitutes the implementation and verification of the computer code generated using field data. The field data used to verify the code is obtained from the U.S. Geological Survey studies conducted for Clinch River at Speers Ferry, VA, Goofrey and Frederick (1970).

6.1 Numerical Examples Group I

The hypothetical problem chosen for these examples can be described as follows: a concentration is introduced to a river reach at a constant rate at a location $x = 0$. The problem consists of the analysis of the convective dispersive transport of this concentration in the positive x-direction with constant uniform rate of flow, $\bar{u}$, with a constant longitudinal dispersion coefficient, D. Initial distribution of this concentration in the reach, $\bar{C}_o$, is assumed to be zero. This problem description is specifically chosen in order to match the conditions descirbed in Section (2.2.E) for which an analytical solution and a corresponding computer code are generated and presented in Appendix I. Thus, the main aim here is to compare the numerical results with the analytical solution and to gain some insight as to the behaviour of the numerical model for various conditions.

The dimensionless form of the time dependent convective diffusion equation and related boundary and initial conditions describing this problem can be given as,

$$\frac{\partial \phi}{\partial \tau} + \lambda \frac{\partial \phi}{\partial \eta} = \frac{\partial^2 \phi}{\partial \eta^2} \qquad (6.1)$$

where

$$\phi = \frac{\bar{C}}{\bar{C}_o}, \ \eta = \frac{x}{L}, \ \lambda = \frac{\bar{u}L}{D}, \ \tau = \frac{Dt}{L^2} \qquad (6.2)$$

where L is the reach length, $\bar{C}_o$ is the initial concentration and other variables are as defined earlier in the report. Several computer runs are generated using the following data

$$0 \leq x \leq 1000 \quad (m)$$
$$D = 20 \quad (m^2/sec)$$
$$\bar{u} = 0.01, 0.02, 0.1, 0.2, 2.0, 10.0 \quad (m/sec)$$

The initial and boundary conditions for this problem can be given as

Initial Condition: $\tau=0$ $\phi=0$

Boundary Condition I: $\eta=0$ $\phi=1$

Boundary Condition II: $\eta=1$ $\frac{\partial \phi}{\partial \eta} = 0$

The region, $0 \leq \eta \leq 1$, is divided into twenty elements for this problem. This results in twenty-one nodes and since $\bar{u}$ and D are constant throughout the region, numerical values for these constants are generated as nodal constants. Execution time for each example on C.D.C. (CYBER) computer was around 0.75 seconds.

Numerical results obtained for these problems are presented in Figures 2-7 simultaneously with the analytical solutions obtained for the same problems. Results clearly indicate that as the magnitude of the coefficient of the convective term, $(\frac{\bar{u}L}{D})$, increases, the numerical solutions become less accurate. A critical case can be seen for $\lambda = 500$ in Figure 7. Such errors are characteristic of computational convection errors. Several studies exist in the literature which analyze the nature and propagation of these errors for several different numerical schemes, Bella (1970) and Holly (1977). At this point we do not intent to go further into the details of numerical error analysis aspects of the suggested computational procedure. Such aspects should be taken up in future studies in order to properly describe the reliability of the model. For lower values of the coefficient, λ, however, the numerical results obtained yield satisfactory results when compared with the analytical solution as seen in Figures 2-6.

The same problem is also extended to a case where the duration of the Boundary Condition I is controlled. Such a case is typical of accidental spills in natural rivers. Results obtained for this case are presented in Figures 8-9. In this problem, Boundary Condition I is altered to $(\eta = 0, \phi = 0)$ for $\tau \geq 0.002$.

6.2 Numerical Examples Group II

Numerical examples included in this group constitute the implementation and verification phase of the study. The patterns of dispersion observed

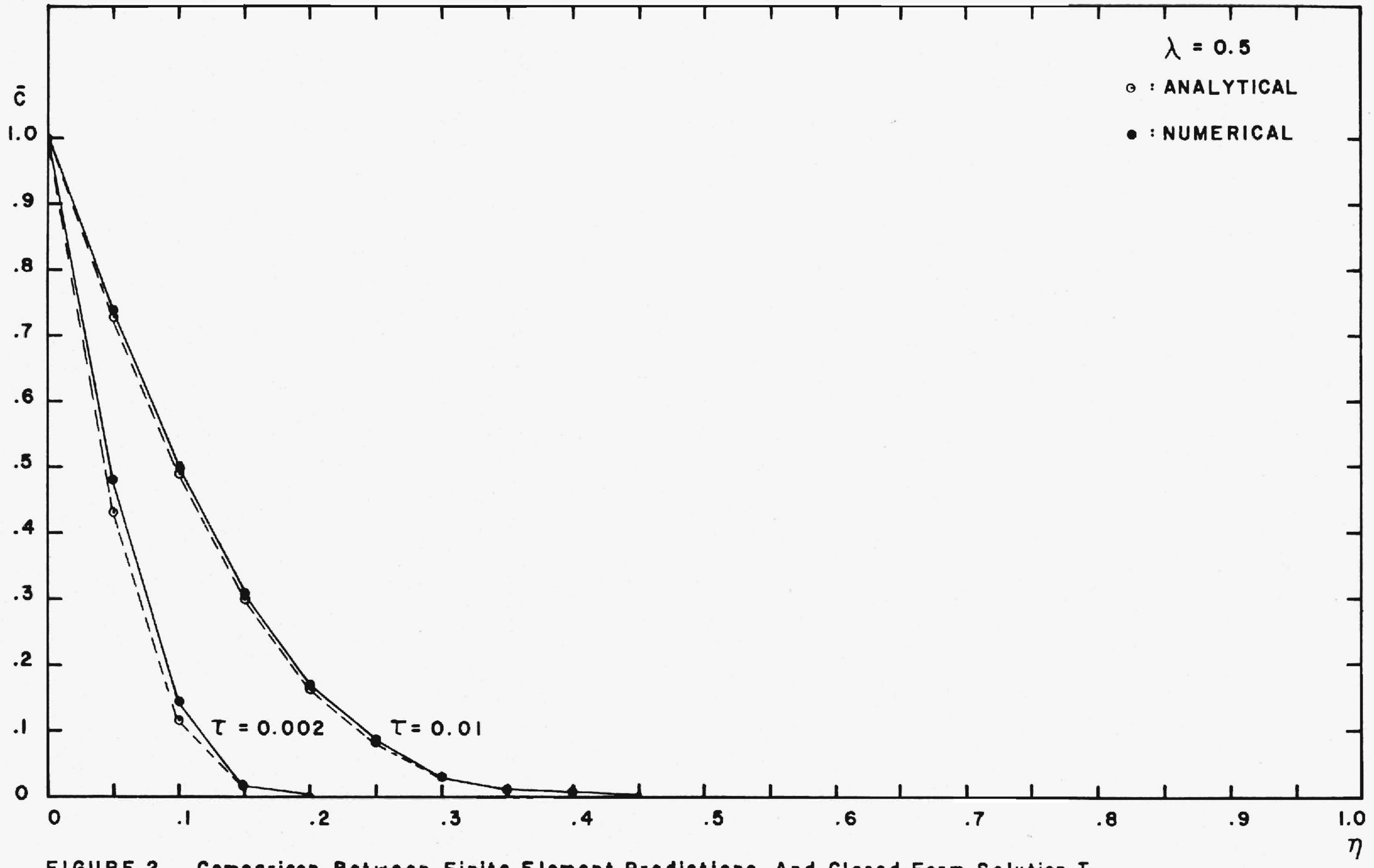

FIGURE 2. Comparison Between Finite Element Predictions And Closed Form Solution I

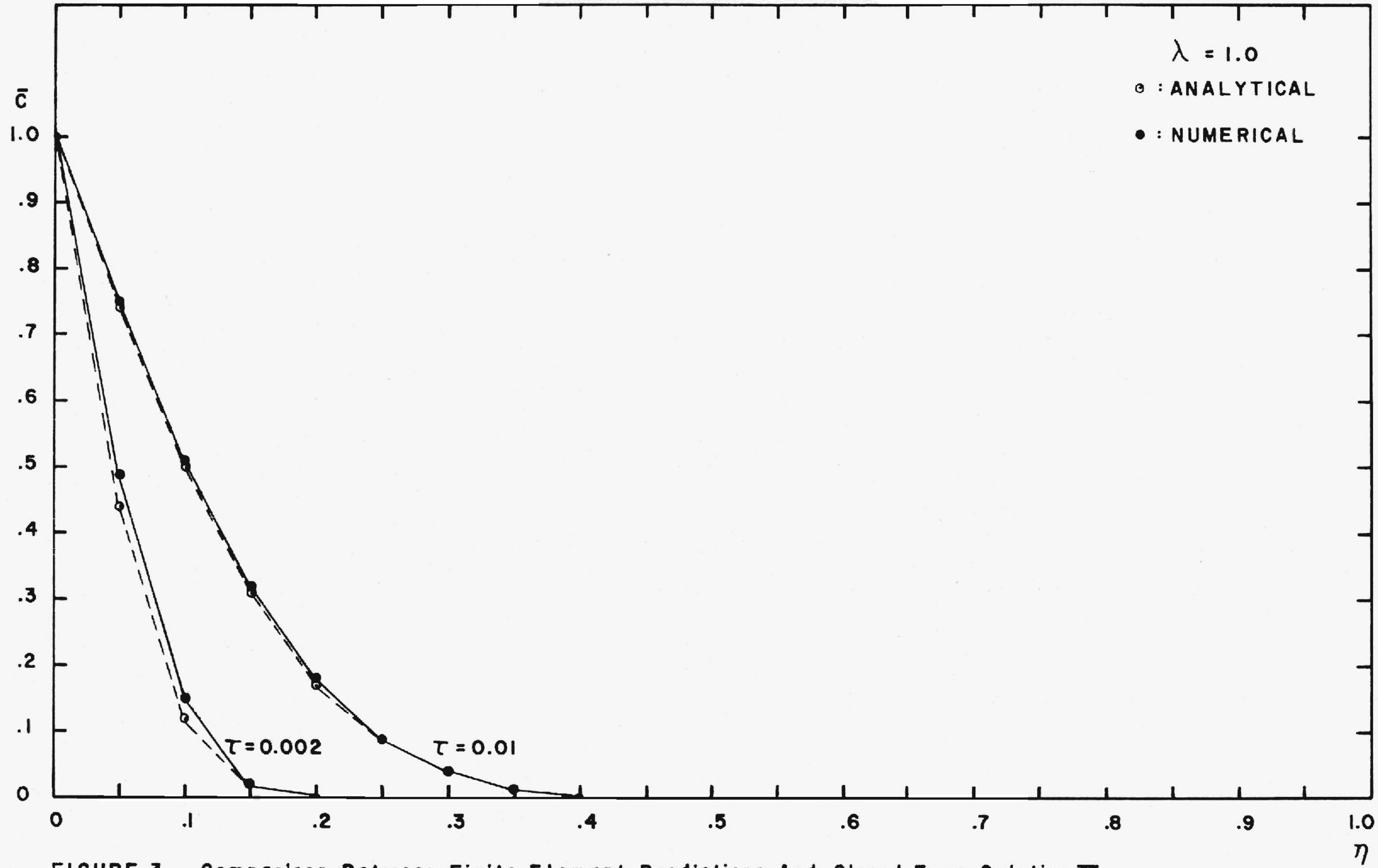

FIGURE 3. Comparison Between Finite Element Predictions And Closed Form Solution II

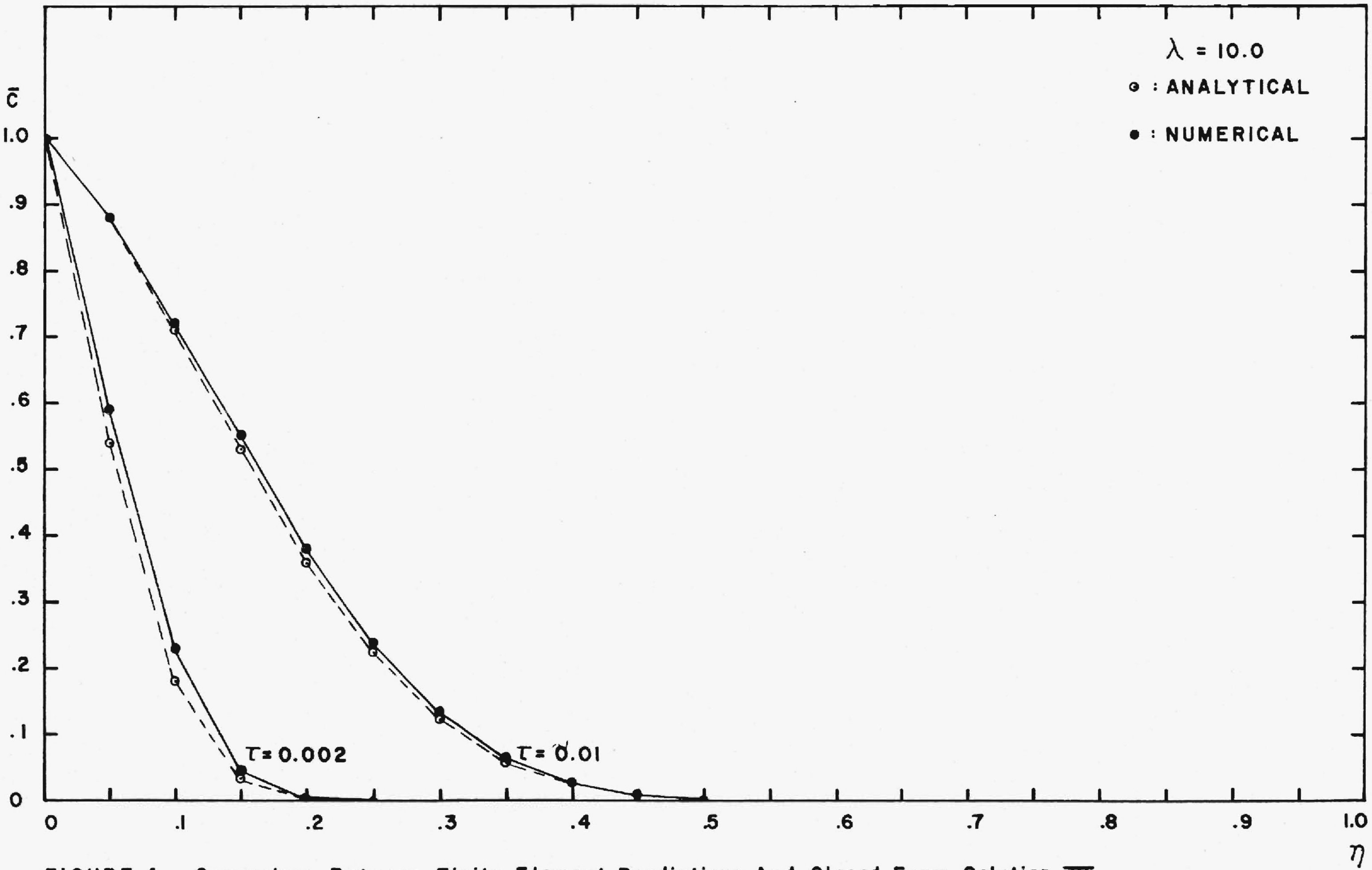

FIGURE 4. Comparison Between Finite Element Predictions And Closed Form Solution III

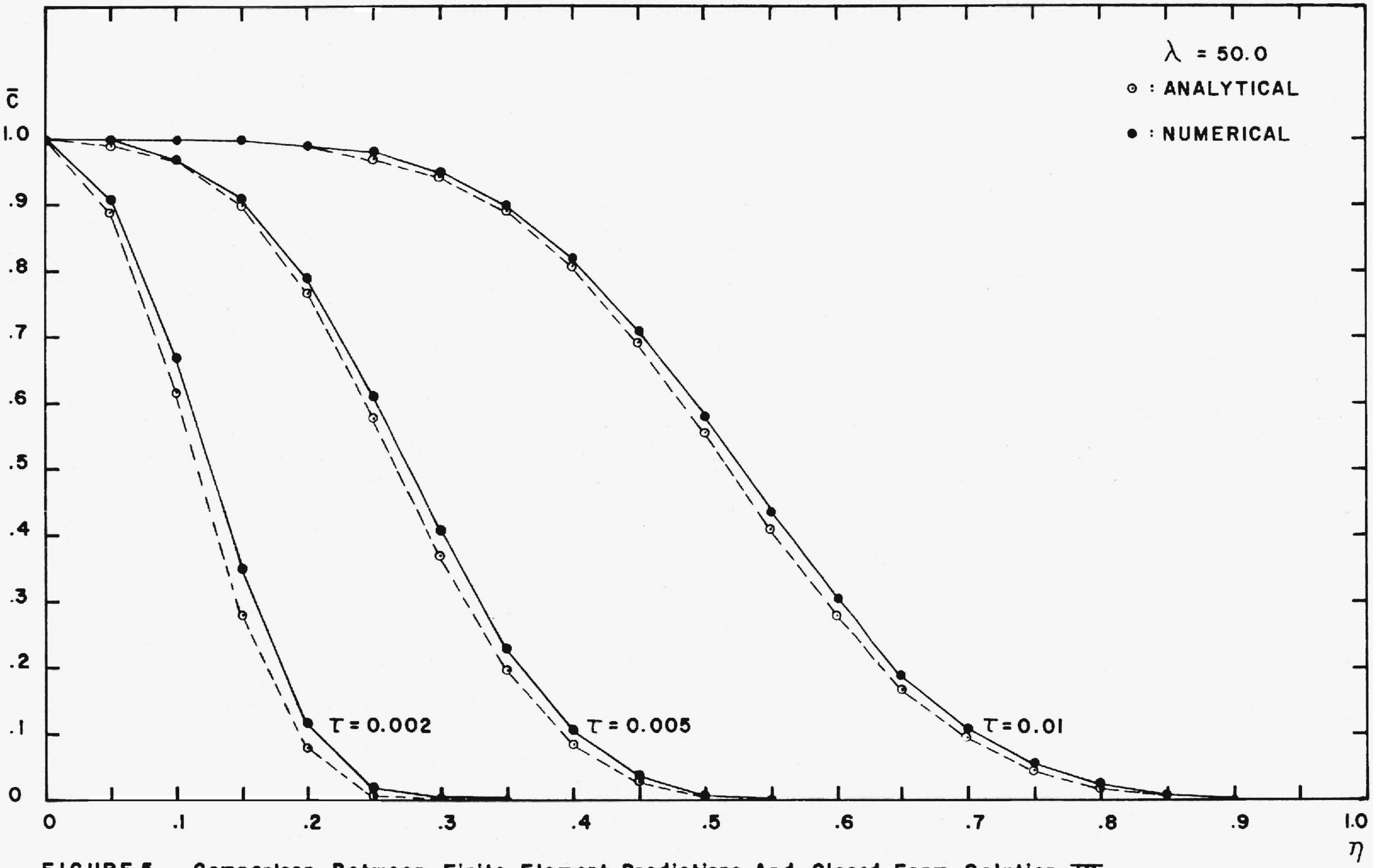

FIGURE 5. Comparison Between Finite Element Predictions And Closed Form Solution IV

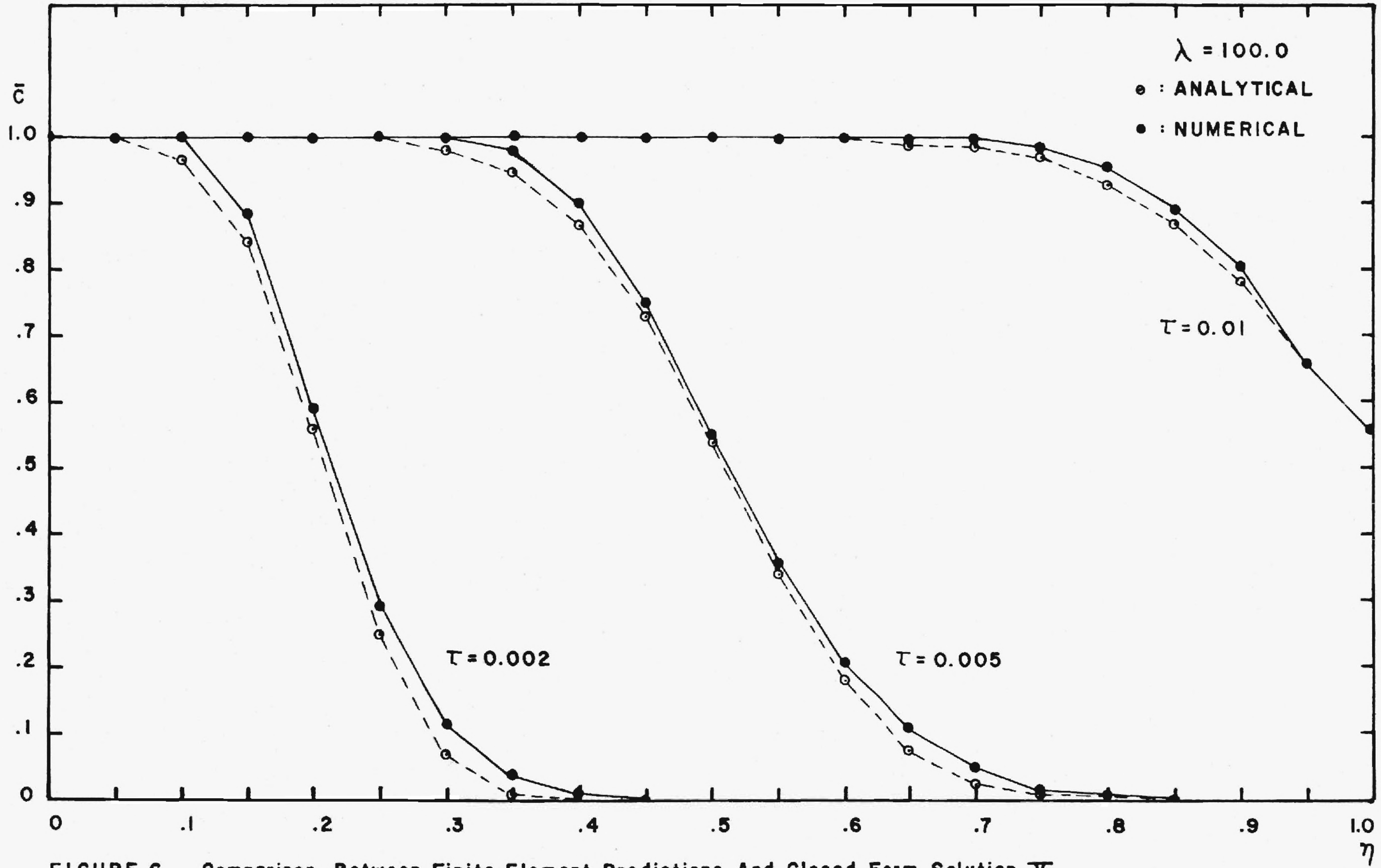

FIGURE 6. Comparison Between Finite Element Predictions And Closed Form Solution V

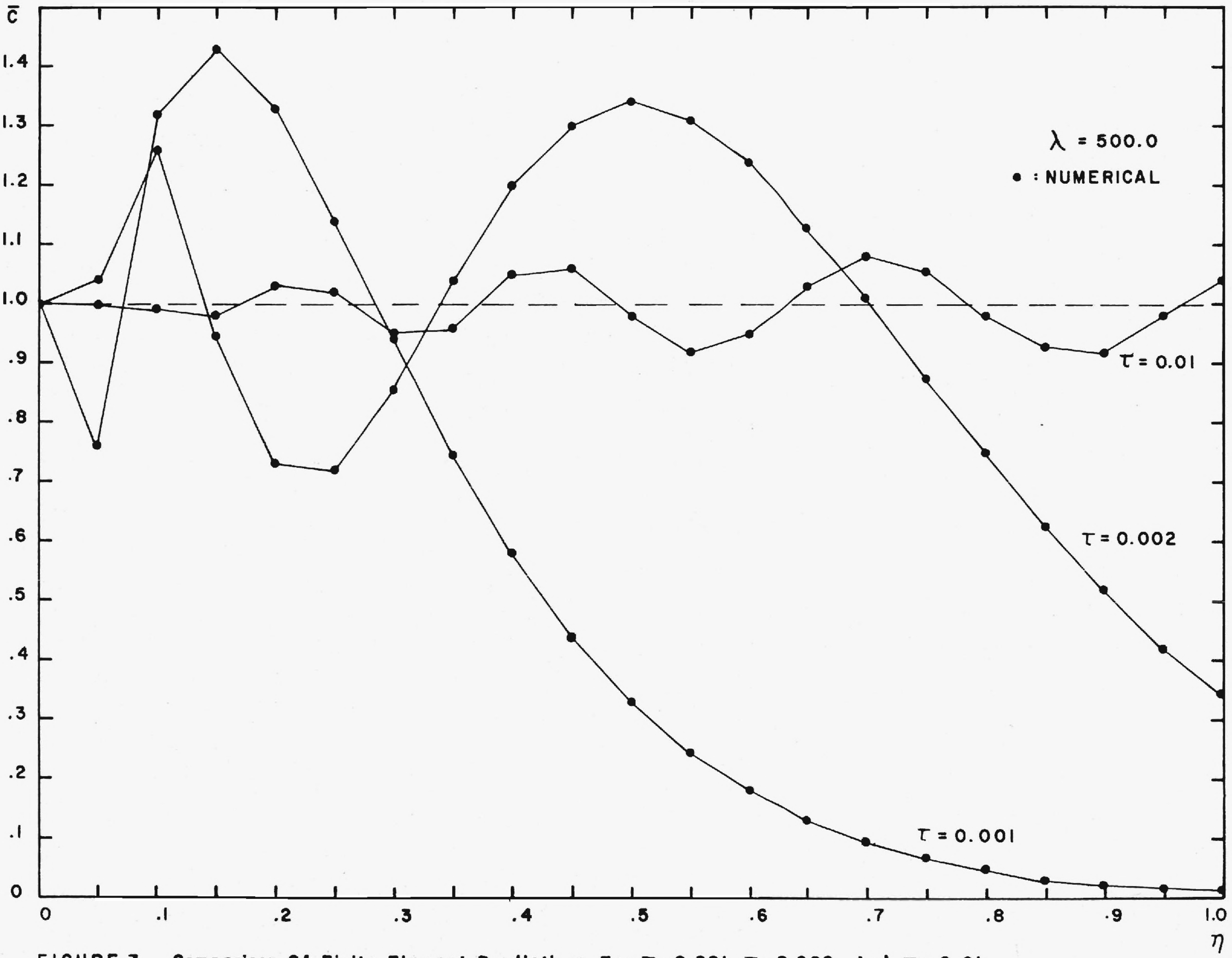

FIGURE 7. Comparison Of Finite Element Predictions For $\tau = 0.001$, $\tau = 0.002$, And $\tau = 0.01$

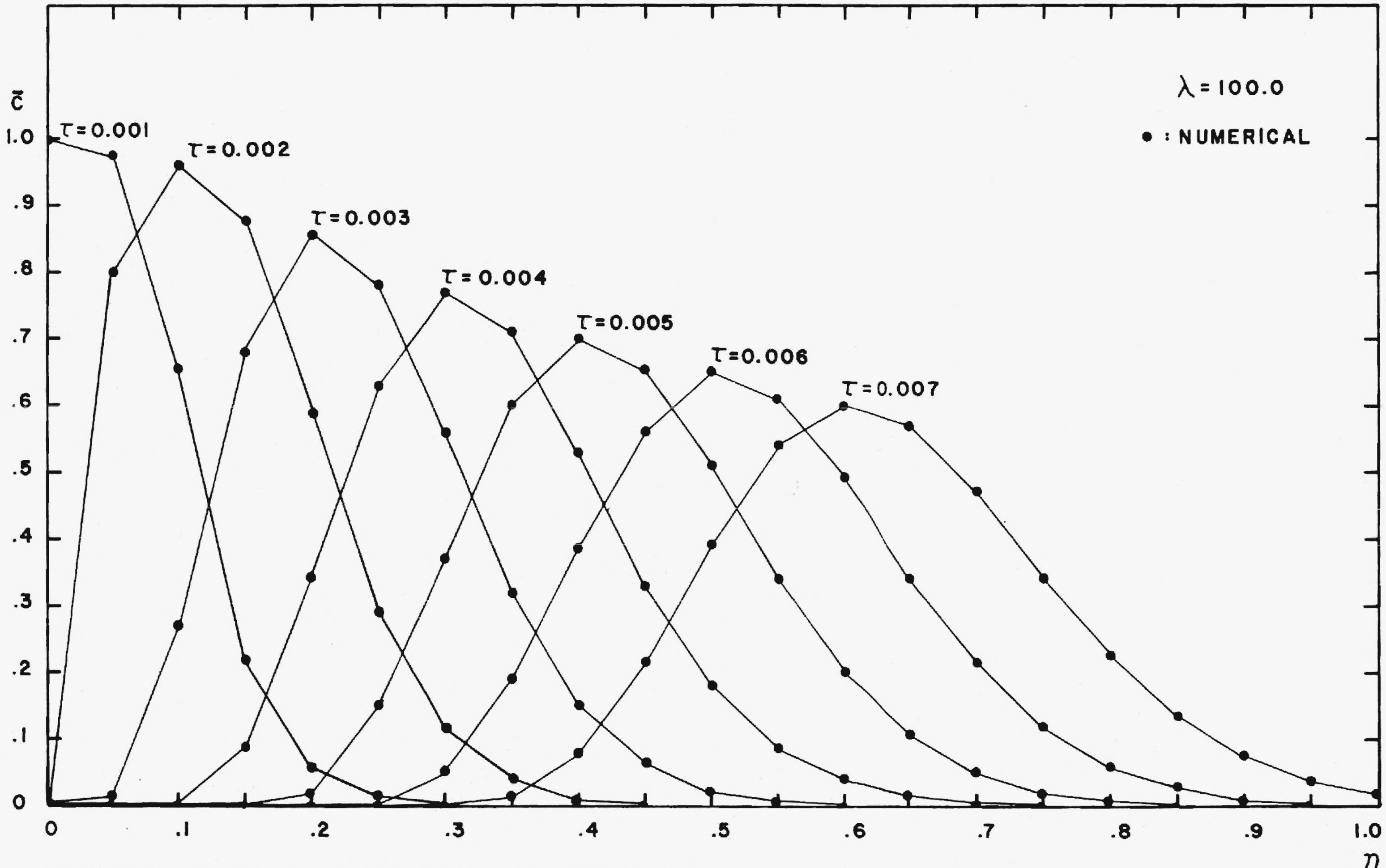

FIGURE 8. Finite Element Predictions For Timed Spill

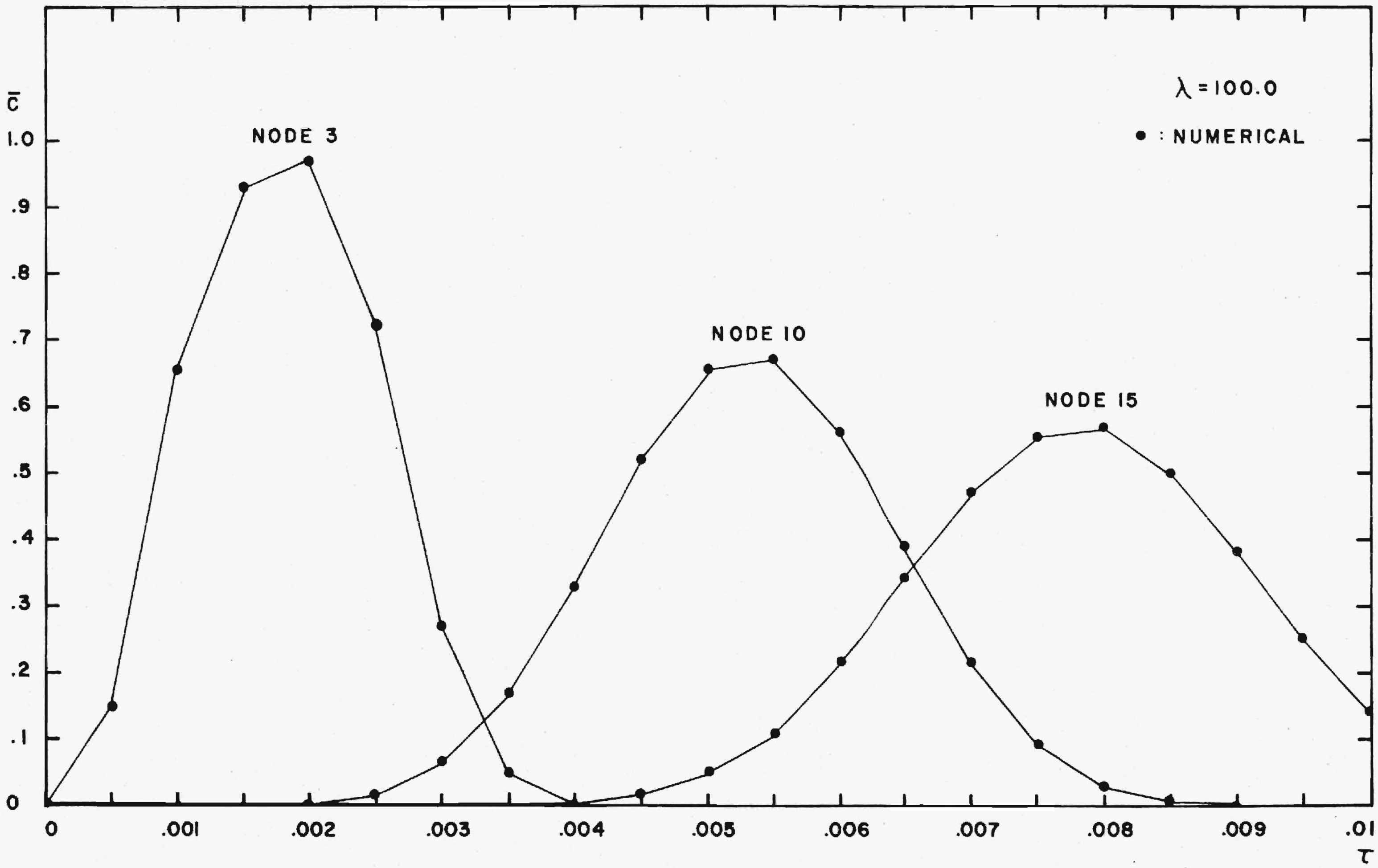

FIGURE 9. Time — Concentration Finite Element Predictions At Nodes 3, 10, And 15 For Timed Spill

by Godfrey and Frederick (1970) at Clinch River, Speers Ferry, VA are compared with patterns predicted by the numerical model developed in this study.

The investigation, referred to above, approached the stream dispersion problem by conducting radiotracer tests in five reaches of natural channels and in one reach of a large irrigation channel. The purpose of these tests was to obtain data for an evaluation of the one dimensional approach to the description of dispersion in large open channels. Throughout the study a critical evaluation of earlier one dimensional models is presented with findings indicating considerable discrepancy with the models of Taylor (1954), Elder (1959), Parker (1958) and Thomas (1958). Of the six reaches where experiments were conducted, Clinch River data was chosen arbitrarily for verification in this study. The alinement of this reach is described as straight with a total length of 5882(m). For each experiment, horizontal and vertical control was established and topographic map of the low-water channel was prepared. Six representative cross sections were chosen in each reach where multiple data collection were made in the same section. The tracer was injected in a line source across the stream either by wading or from a boat. About 15 milliliters of the tracer, a highly concentrated solution of gold chloride in nitric and hydrochloric acid, was diluted to a volume of 2 liters using water from the stream to minimize the difference in specific gravity between the tracer and the stream. The injection was started several meters from one bank and stopped short of the opposite bank, to minimize the contamination of banks by the injected solution. The injection was made at a uniform rate over a 1 minute period. The concentration of radionuclide used in each test was proportional to the discharge, about 2 millicuries per cubic foot per second. Gold-198 was selected as the radiotracer because of high permissible concentrations, short half-life and low cost. The concentrations of the activity in the stream were observed by a scintillation detector with a one-by-one inch sodium iodide thallium-activated crystal. The concentrations were measured at or near the center-line of the stream. Detailed statistics of the experimental data for the Clinch River test can be seen in Table 6.2-1.

The data for the numerical model are generated using these base data. The reach is divided into seven subreaches with each subreach beginning and ending with the station location designated in the experimental setup. Each subreach is divided into smaller elements with (30), (40), (40), (50), (50), (60) and (10) elements, consecutively, from the point of injection to the extended end of the reach. This idealization resulted in (280) elements with (281) nodes. In each subreach the velocities and disperion coefficients are assumed to be constant with varying magnitudes from subreach to subreach. Five computer runs are made for this set up in order to observe the behavior of different aspects of the model generated. In the first run, decay of tracer element is ignored and the longitudinal dispersion coefficient is introduced as input data using the value estimated in the experimental study. The longitudinal dispersion coefficient was predicted to be 11.0 m^2/sec for the Clinch River reach near Speers Ferry, VA. In Figure 10, observed time concentration data at five stations are plotted against the computed time concentration values at the same stations. The agreement between the model results and experimental data is excellent. Prediction of arrival time of peak concentrations at stations one, two, three, and four are excellent

TABLE 6.2-1

CHANNEL GEOMETRY, FLOW DATA AND STATISTICAL PARAMETERS FOR CLINCH RIVER TEST

Section	1	2	3	4	5	6
x (m)	688.84	1575.80	2490.22	3596.64	4663.44	5882.64
Width (m)	60.96	50.29	48.76	55.78	53.34	50.59
Depth (m)	1.74	1.62	1.98	2.26	2.25	2.72
R (m)	1.69	1.60	1.95	2.20	2.20	2.66
Fall (m)	0.70	1.25	1.42	1.62	1.98	2.24
Temp. ^{o}F	67.0	67.0	67.0	68.0	68.0	68.0
Q (m^3/s)	85.81	79.86	89.20	86.94	83.83	85.24
$\bar{u}$ (m/s)	0.81	0.98	0.92	0.68	0.70	0.62
$\bar{t}$ (sec)	684.00	1730.00	3070.00	4570.00	5740.00	8940.00
U_* (m/s)	0.13	0.11	0.103	0.09	0.09	0.103

Note : $\bar{t}$: Elapsed time for the centroid of tracer cloud to move the distance (x) in seconds.

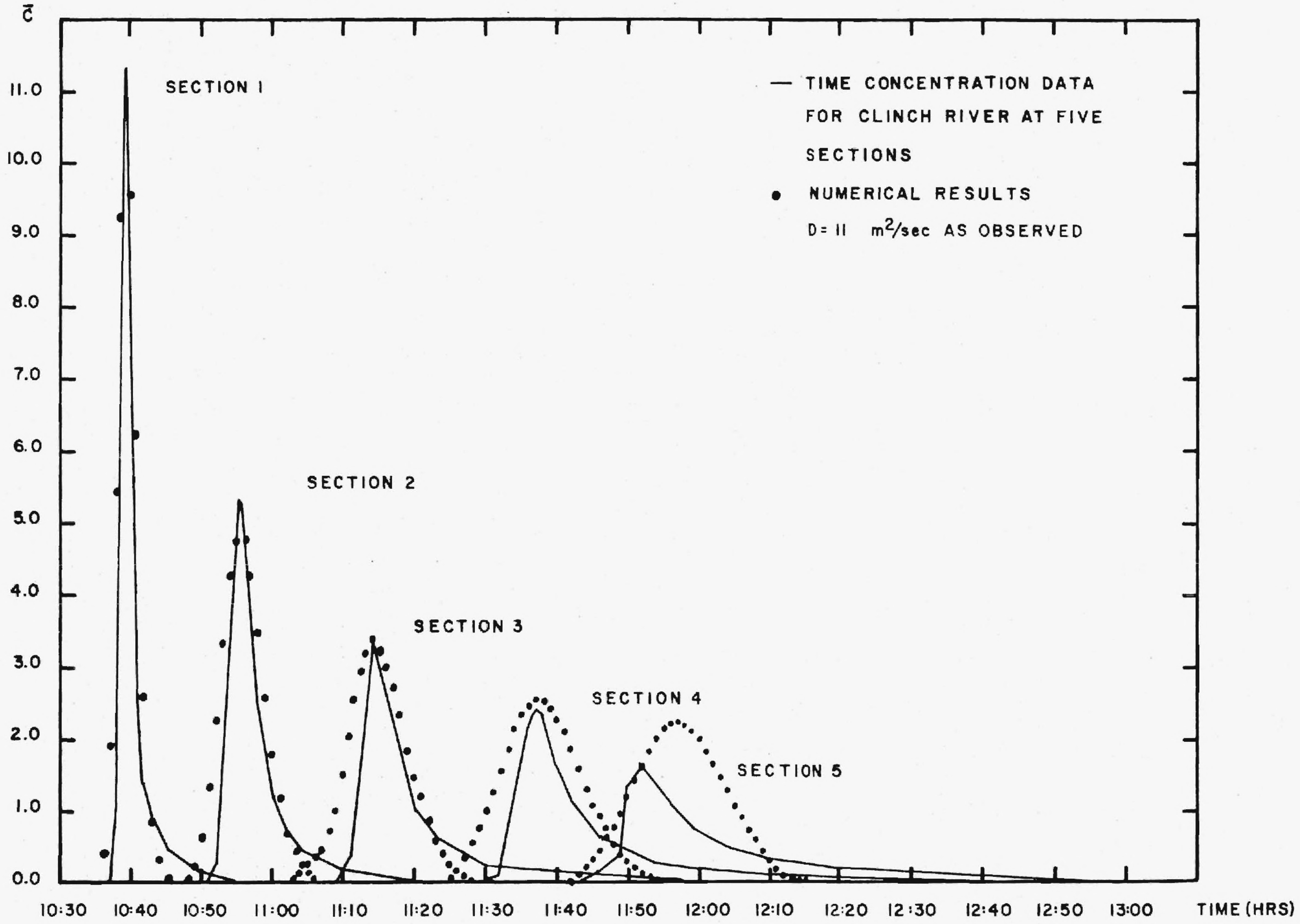

FIGURE 10. Time – Concentration Data And Numerical Results I

with a four minute lag in station five. The concentration intensities predicted by the model are within 3% for the predicted peak concentration intensities at each station. The numerical results seem to diverge from the observed values as the tracer is transported in the downstream direction. This is expected however since decay of the Gold-198 element is not considered in this run. Overall results obtained in this run are satisfactory with the model yielding conservative estimates.

In order to observe the effects of decay of the tracer element used, this computer run is repeated including the decay of Gold-198, (half-life: 64h). Results are presented in Figure 11 in the same manner as before. The agreement between the numerical results and observed data for this case is excellent for peak concentrations. For the both tails of concentration distribution at a station, however, the model predicts much shorter durations with the difference becoming larger as the tracer is transported in a downstream direction.

In the third, fourth and fifth runs, the longitudinal dispersion coefficient is predicted in each subreach using the quations described in Section 3. The first prediction is done using the Equation (3.5) which was developed in this study. Results obtained for each reach and predictions of time concentration values at each station are given in Figure 12 comparatively with the observed data. Due to higher dispersion coefficients predicted, the tracer arrives more dispersed to the stations in downstream sections with lower peak values. Time of arrival of the peak is also shifted to the left indicating an early arrival. All these changes are expected numerically since higher longitudinal coefficients used in each reach would tend to distort the results in this manner. Once again this computer run stresses the

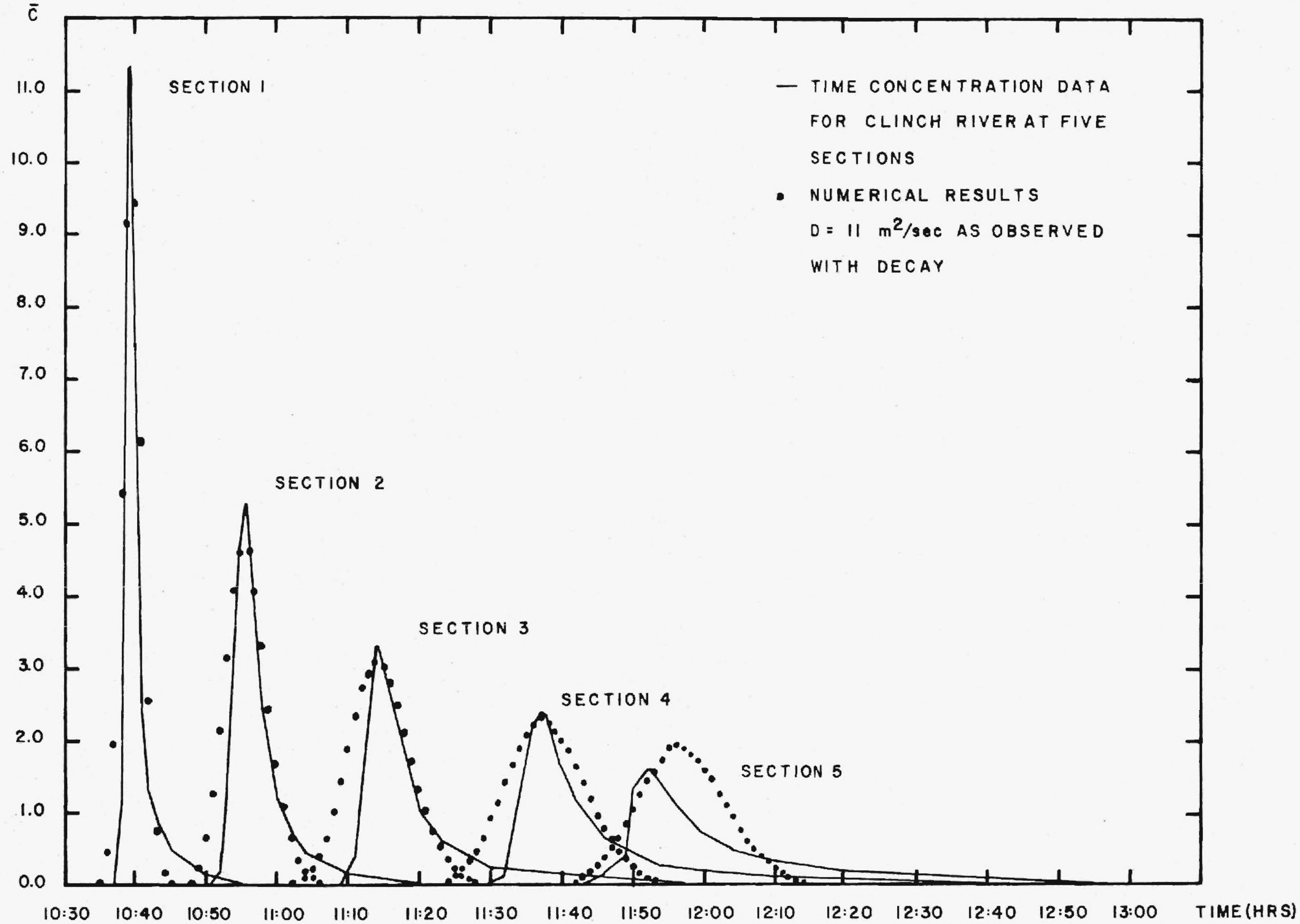

FIGURE 11. Time–Concentration Data And Numerical Results II

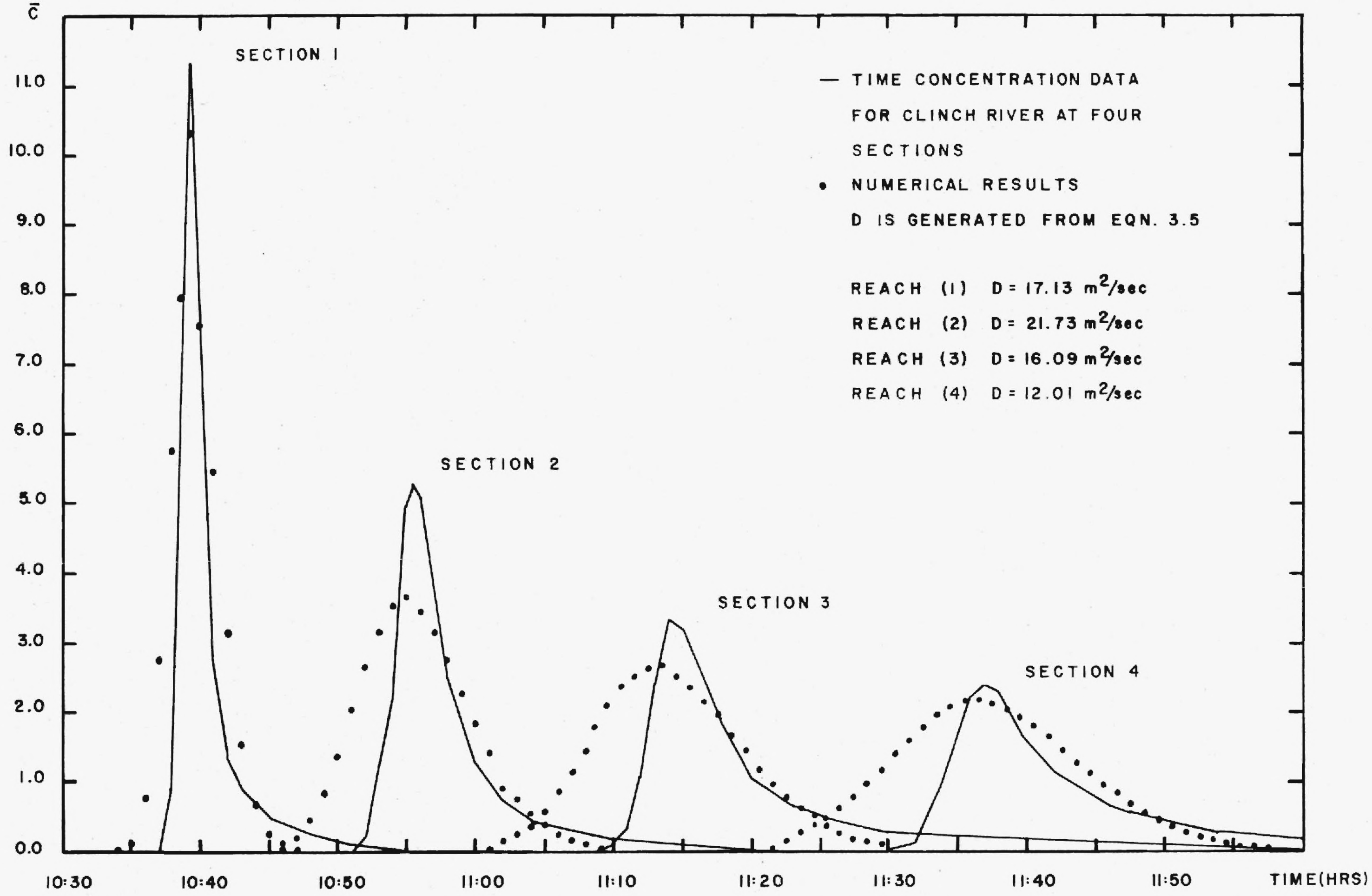

FIGURE 12. Time—Concentration Data And Numerical Results III

importance of the longitudinal dispersion coefficient. In this and the following runs decay of the tracer element was ignored.

In the two remaining runs, the longitudinal dispersion coefficient was predicted using Equations (3.2) and (3.1) of Section 3. Since the resulting dispersion coefficients were larger for these cases the predicted values for concentration intensities were much more dispersed in comparison to the first case. Numerical results for these two runs are presented in Figures 13 and 14 comparatively with the observed data, indicating again the importance of the longitudinal dispersion coefficient.

The five computer runs presented in this last group of examples clearly indicate that the model is capable of predicting mass transport in a natural river extremely accurately if proper values of field parameters are used as base data. The prediction of these field parameters, however, is crucial in such analysis and more detailed studies should be performed to arrive at better predictive equations. The Equation suggested in this study for this purpose definitely seems to be a better model than the other two which are obtained from most recent studies in the related literature. The predictive Equation (3.5) should be considered as a first step towards a better description of longitudinal dispersion in natural rivers.

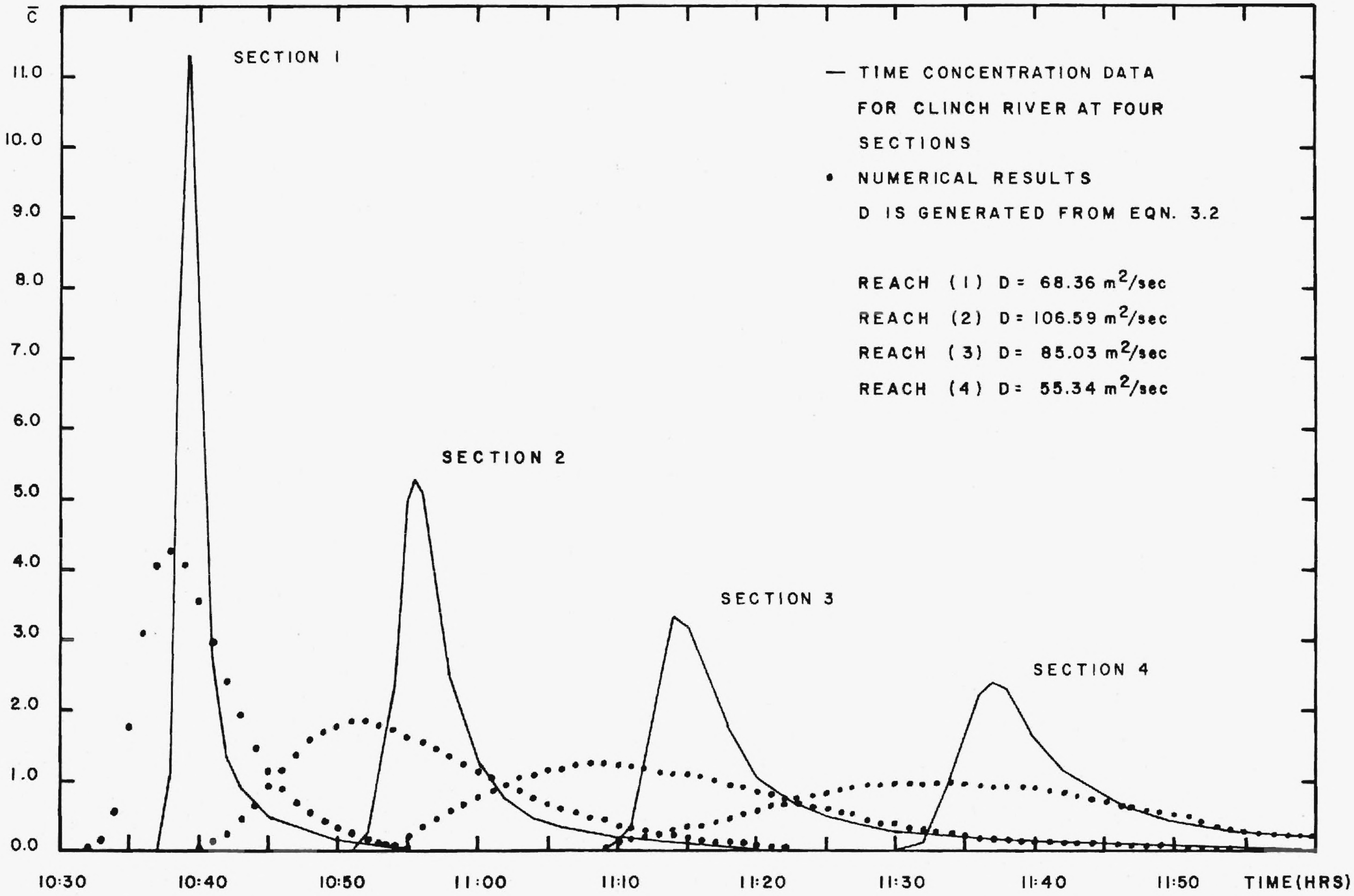

FIGURE 13. Time – Concentration Data And Numerical Results IV

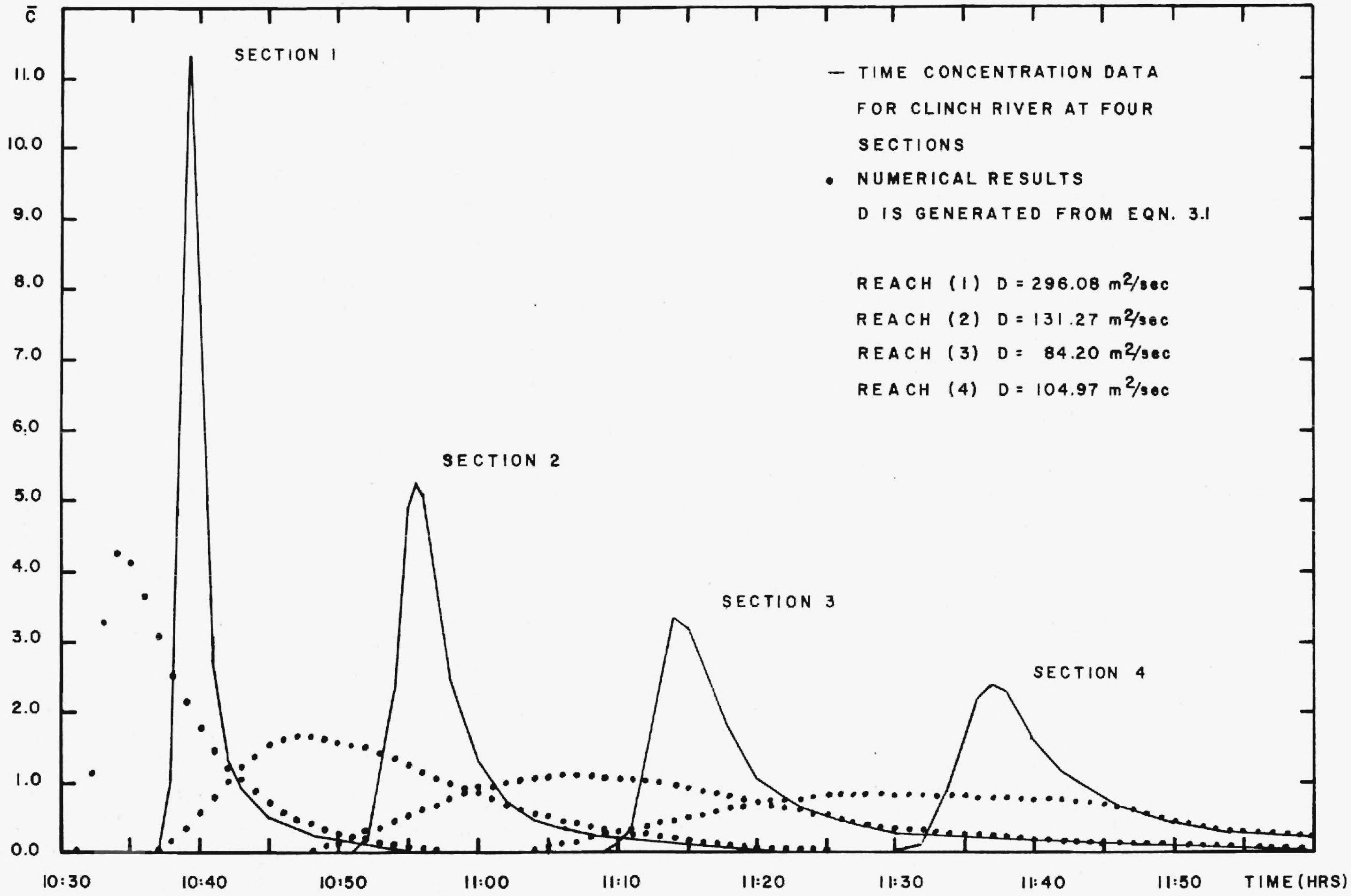

FIGURE 14. Time—Concentration Data And Numerical Results V

7.0 CONCLUSION

This study was planned and carried out as an initial step in modeling mass transport in natural rivers. Throughout, the aim was to develop a simple user oriented numerical model which can be used in the analysis of such mass transport problems. The short time period of the study naturally imposed certain limitations on the properties of the resultant model, which are summarized below. The evaluation and employment of the model have to be within the bounds of these limitations.

The purpose of the present model is to obtain initial estimates of concentration distribution of a pollutant, at the downstream sections of a river reach, following an accidental spill. Since one of the most important benefits of developing such a model involves its being used in emergency situations, the model should be well documented, readily available and should require a minimum data preparation effort for implementation. These considerations have dictated the direction of work on the present model.

The computer code generated, its documentation and steps involved in data preparation are summarized in detail in previous sections of this report. The construction of the model is such that, in addition to certain finite element data generation short cuts, certain field parameters are estimated by the model itself while others have to be fed in as input data. The parameters estimated by the model are the decay constants of several radionuclides and the diffusion coefficient. The kinematic parameters of the river reach and other physical parameters related to the river reach are treated as input data. No attempt was made to extend the model so as to estimate the latter set of parameters at this stage, since the present model was intended as a rather simple, initial device.

In the preparation of the program, one of the considerations was to render data preparation as uncomplicated as possible for the users' convenience. As described in Section 5, the data preparation required for the present model is rather simple and straightforward. Nevertheless, if and when the extensions suggested here are incorporated into the model, data preparation will be further minimized and simplified.

In its present form, as discussed in Section 6, the model developed here provides conservative, reliable and reasonable estimates of pollutant concentration intensities in field applications. Although the model performs rather well within the bounds of the limitations imposed on the study from its conception, it is important to recognize the nature of these limitations and their implications for the potential usefulness of the model. To repeat, the present model should be considered only an initial step in the modeling of convective dispersive mass transport in natural rivers. Its extension in various directions is both possible, and necessary to obtain a more realistic and safe to use version. Below we discuss some of these limitations and related possible extensions.

We have stated above that concentration intensities predicted by the model are conservative. The degree of conservativeness of these estimates are naturally limited by the assumptions made in the construction of the model. For example, absorbtion by sediments and vegetation uptake are ignored in the present model. In reality, in most rivers such processes do take place, leading to concentration build-up. Thus, the true values of the concentration distribution will be greater than the values estimated through the use of the model generated in this study. In this sense, then, the estimates resulting from the use of the model would not be conservative and such use would not provide optimum safety in emergency situations which involve potential environmental and/or health hazards. Therefore, it is extremely important that the present model be extended to allow for the incorporation of uptake and absorption phenomena.

Apart from the safety related considerations discussed above, the model has other, more elementary deficiencies which can and should be eliminated through future work. The first of these extensions should be the development of a subprogram, to be added to the existing program, which would predict the values of the kinematic parameters within the body of the model itself. Such an addition will eliminate the necessity for the user to prepare the values of the kinematic parameters at various locations in a reach as input data. Such an extension will make the study of regulated rivers possible which is a major drawback of the present model. The required input data will then consist of only initial and boundary conditions at several locations over the reach.

The second possible extension involves modeling of branching river networks. As it stands now, the model is valid for the analysis of mass transport phenomena in a single reach.

Thirdly, future work on the modeling of convective diffusion equation should include more detailed analyses of numerical accuracy. In depth study of numerical accuracy in both the present model and in those to be developed in the future will prove to be very helpful in relation to safety considerations involved in decision making regarding potential areas of use. In this context, it is necessary to obtain numerical error bounds for all such models.

Finally, in the present model transport of a single element is taken into consideration. Future work could incorporate the behavior of two or more interacting elements yielding a more realistic model.

The discussion up to now has been on the potential extensions of the basic one dimensional model. Once the one dimensional model is perfected, the next step would involve the development of a two dimensional model of mass transport in natural rivers. All of the above considerations can then be incorporated into the two dimensional model. The basic aim throughout is the construction of user oriented "simple" models rather than those portraying fancy numerical procedures. This last point is significant in considering whether or not the development of three dimensional models should then be attempted. The state-of-the art in numerical analysis at the present time would allow the construction of three dimensional models of mass transport in natural rivers. However, it is well known that for many of the physical phenomena involved in river flow, no proper description in physical and mathematical terms is yet available. Since the accuracy of resultant estimates obtained through the application of models are in a very basic sense limited by the accuracy of the description of these phenomenon, at this stage the construction of three dimensional models in natural rivers would provide no additional utility other than academic satisfaction.

To conclude, the results of this study clearly indicate that it is possible to generate regional package programs to predict pollution transport in a river reach. These package programs will provide sufficiently reliable initial estimates of concentration intensity in a sufficiently short time to be helpful for many environmental and health safety considerations. The potential utility of such package programs for the various purposes and needs of the various agencies involved in related areas could not be exaggerated.

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A P P E N D I X I

PROGRAM NAME : CONCEN

This program computes the Equation (2.33) which is the analytical solution to the problem described in section 2.2.E.

Input Data :

Input data should be entered using the NAMELIST type format.

Variables :

NROOT	:	Number of roots desired
CO	:	Initial concentration
D	:	Diffusion coefficient
U	:	Velocity
XI	:	Initial length
XF	:	Final length
XST	:	Length increment
TI	:	Initial time
TF	:	Final time
TST	:	Time step

```
      PROGRAM CONCEN(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION  ALAM(100), ALPHA(100), AA(100)
      NAMELIST/DATA1/ NROOT,D,U,CO
      NAMELIST/DATA2/ XI,XF,XST,TI,TF,TST

      READ(5,DATA1)
      READ(5,DATA2)
      WRITE(6,100) NROOT,CO,D,U,XI,XF,XST,TI,TF,TST
      DO 10 I = 1,NROOT
      ALAM(I) = ROOT(XF,D,U,I)
      ALPHA(I) = ALPH(U,D,ALAM,I)
      AA(I) = A(CO,U,D,XF,ALAM,I)
   10 CONTINUE

      DO 20 I = 1,NROOT
      WRITE(6,110) ALAM(I), ALPHA(I), AA(I)
   20 CONTINUE

      TCONT = TI + TST
   30 CONTINUE
      ISIG = 0
      XCONT = XI + XST
      WRITE(6,120) TCONT
   40 CONTINUE
      SUMC = 0.00
      DO 50 I = 1,NROOT
      SUMC = SUMC + AA(I) * EXP(-ALPHA(I)*TCONT) * SIN(ALAM(I)*XCONT /
     1       (2.0*D))
   50 CONTINUE
      CONC = CO + EXP(U * XCONT / (2.0*D)) * SUMC
      IF(CONC .LT. 0.00) ISIG = 1
      IF(ISIG .EQ. 1) CONC = 0.00
      WRITE(6,130) XCONT, CONC

      XCONT = XCONT + XST
      IF(XCONT .LT. XF) GO TO 40

      TCONT = TCONT + TST
      IF(TCONT .LT. TF) GO TO 30

  100 FORMAT(1H1,///,37X,*INPUT DATA*,///,10X,*NROOT =*,I3,5X,
     1*CO =*,E15.6,5X,*D =*,E15.6,5X,*U =*,E15.6,//,
     210X,*XI =*,E15.6,5X,*XF =*,E15.6,5X,*XST =*,E15.6,//,
     310X,*TI =*,E15.6,5X,*TF =*,E15.6,5X,*TST =*,E15.6,///)
  110 FORMAT(8X,*ALAM(I) =*,E15.6,5X,*ALPHA(I) =*,E15.6,5X,*AA(I) =*,
     1E15.6)
  120 FORMAT(///,19X,*TCONT =*,E15.6,//)
  130 FORMAT(8X,*XCONT =*,E15.6,5X,*CONC =*,E15.6)

      STOP
      END
      FUNCTION ROOT(XF,D,U,I)

      X = I
      ROOT = 3.1416 * X
      DO 10 J = 1,20
      ROOT = ATAN(-2.*D/(XF*U)* ROOT) + 3.1416 *X
   10 CONTINUE
      ROOT = ROOT*2.*D/XF
      RETURN
      END
      FUNCTION ALPH(U,D,ALAM,I)
      DIMENSION ALAM(100)
```

```
ALPH = (U*U + ALAM(I)*ALAM(I)) / (4.0*D)
RETURN
END
FUNCTION A(CO,U,D,XF,ALAM,I)
DIMENSION  ALAM(100)

X = -4.0*CO*D*ALAM(I)*ALAM(I)
Y = U*U + ALAM(I)*ALAM(I)
Z = XF*ALAM(I) - D*SIN(ALAM(I)*XF/D)

A = X / (Y * Z)
RETURN
END
```

PROGRAM NAME : DECAY1D

This program computes the Equation (2.28) which is the analytical solution to the problem described in section 2.2.D.

Input Data :

Input data should be entered using the NAMELIST type format.

Variables :

ITIME : Time indicator (0 or 1)
UF : Velocity
ES : Diffusion constant
XKD : Decay constant
XL : Total length
DX : Length increment
TI : Initial time
TF : Final time
TST : Time step

```
      PROGRAM DECAY (INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)

      COMMON/CONST/ ITIME,LCOUNT,UF,ES,XKD,XL,DX,CS,X
      COMMON/TME/ TI,TF,TST,TCONT

      NAMELIST/DATA1/ ITIME,UF,ES,XKD,XL,DX
      NAMELIST/DATA2/ TI,TF,TST

      LCOUNT = 1
      READ(5,DATA1)
      IF(ITIME .EQ. 1) READ(5,DATA2)
      CALL OUTPUT
      IF(ITIME .EQ. 0) CALL STEADY
      IF(ITIME .EQ. 1) CALL TIME
      STOP
      END
      FUNCTION ERF(X)
      ERF = 2.0 / SQRT(3.141593) * (X - X**3/3.
     1      + X**5/(2.*5.) - X**7/(3.*2.*7.)
     2      + X**9/(4.*3.*2.*9.) - X**11/(5.*4.*3.*2.*11.)
     3      + X**13/(6.*5.*4.*3.*2.*13.) )
      RETURN
      END
      SUBROUTINE STEADY

      COMMON/CONST/ ITIME,LCOUNT,UF,ES,XKD,XL,DX,CS,X

      LCOUNT = 2
      X = 0.00
      OMEGA = SQRT(UF * UF + 4. * XKD * ES)
      X = X + DX
   10 CONTINUE
      CS = 1.0 / OMEGA * EXP((X/2.0*ES) * (UF-OMEGA))
      CALL OUTPUT
      X = X + DX
      IF(X .LE. XL) GO TO 10
      RETURN
      END
      SUBROUTINE TIME

      COMMON/CONST/ ITIME,LCOUNT,UF,ES,XKD,XL,DX,CS,X
      COMMON/TME/ TI,TF,TST,TCONT

      TCONT = 0.00
      OMEGA = SQRT(UF * UF + 4. * XKD * ES)
      TCONT = TI + TST
   10 CONTINUE
      LCOUNT = 3
      CALL OUTPUT
      X = 0.00
      X = X + DX
   20 CONTINUE
      PP = (X + OMEGA * TCONT) /(SQRT(4. * ES * TCONT))
      PM = (X - OMEGA * TCONT) /(SQRT(4. * ES * TCONT))
      ERFP = ERF(PP)
      ERFM = ERF(PM)
      CS = 0.5 * EXP(X * UF/(2. * ES)) * ((ERFP - 1)
     1      * EXP(X * OMEGA / (2. * ES)) - (ERFM - 1)
     2      * EXP(-X * OMEGA / (2. * ES)))
      LCOUNT = 4
      CALL OUTPUT
      X = X + DX
      IF(X .LE. XL) GO TO 20
      TCONT = TCONT + TST
```

```
      IF(TCONT .LE. TF) GO TO 10
      RETURN
      END
      SUBROUTINE OUTPUT

      COMMON/CONST/ ITIME,LCOUNT,UF,ES,XKD,XL,DX,CS,X
      COMMON/TME/ TI,TF,TST,TCONT

      GO TO (10,20,30,40) LCOUNT
   10 CONTINUE
      WRITE(6,100)
      WRITE(6,110)
      WRITE(6,120) UF,ES,XKD,XL,DX
      IF(ITIME. EQ. 1) WRITE(6,130) TI,TF,TST
      GO TO 1000
   20 CONTINUE
      IF(X .EQ. DX) WRITE(6,140)
      WRITE(6,150) X,CS
      GO TO 1000
   30 CONTINUE
      IF(TCONT .EQ. TI + TST) WRITE(6,160)
      WRITE(6,170) TCONT
      GO TO 1000
   40 CONTINUE
      WRITE(6,150) X,CS

  100 FORMAT(1H1)
  110 FORMAT(4(/),51X,*ONE-DIMENSIONAL DECAY EQUATION*,/,
     156X,*ANALYTICAL SOLUTION*,///,61X,*INPUT DATA*)
  120 FORMAT(//,15X,*UF=*,1PE12.5,5X,*ES=*,E12.5,5X,*XKD=*,E12.5,5X,
     1*XL=*,E12.5,5X,*DX=*,E12.5)
  130 FORMAT(//,38X,*TI=*,1PE12.5,5X,*TF=*,E12.5,5X,*TST=*,E12.5)
  140 FORMAT(1H1,4(/),55X,*STEADY STATE SOLUTION*,///)
  150 FORMAT(49X,*X=*,1PE12.5,5X,*CS=*,E12.5)
  160 FORMAT(1H1,4(/),54X,*TIME DEPENDENT SOLUTION*)
  170 FORMAT(3(/),57X,*TCONT=*,1PE12.5,//)

 1000 CONTINUE
      RETURN
      END
```

A P P E N D I X II

```
      PROGRAM IRMOD(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION TITLE(20),S(1000,3),P(1000,3),R(1000),X(1000),
     2SE(2,2),PE(2,2),RE(2),DX(1000),U(1000),GAMA(1000),CIN(1000)
     3,NBCN(5),BCN(5),NDBCN(5),BCD(5),NMBCN(5),BCM(5),G(1000)
      DIMENSION RBN(1000),CC(1000,3)
      COMMON/CHR/ NNODE,NELEM,MAT
      COMMON/ELM/DXX,UU,FF,U1,U2,DX1,DX2,F1,F2,GG,G1,G2
      COMMON/DATA/DX,U,GAMA,X,G
      COMMON/MVEL/ SE,RE,PE,AL,II
      COMMON/BC/NBCN,BCN,NDBCN,BCD,NMBCN,BCM
      COMMON/CONS/ISEC,ITIME,IDXGEN,NNBC,NDBC,NMBC,IP,IGAMG,IUNIT
      COMMON/GMV/S,R,P,CIN
      COMMON TITLE,TI,TF,TST,TCONT,TD
      READ(5,1) ISEC,ITIME,NNBC,NDBC,NMBC,IGAMG
    1 FORMAT(8I2)
      WRITE(6,2)
    2 FORMAT(///10X,"THIS PROGRAM WAS PREPARED AND SUBMITTED IN PARTIAL
     2FULFILLMENT OF PROJECT NO: E20-604",//,10X,"BETWEEN EMORY UNIVERSIT
     3Y AND GEORGIA INSTITUTE OF TECHNOLOGY, ATLANTA GEORGIA")
      WRITE(6,3)
    3 FORMAT(/10X,"THE PROGRAM IS PREPARED BY DR. MUSTAFA M. ARAL OF GEO
     2RGIA INSTITUTE OF TECHNOLOGY, SCHOOL OF CIVIL ENGINEERING",//,10X,
     3"THE PROGRAM IS THE OUTCOME OF A PRELIMINARY STUDY DONE FOR OAK RI
     4DGE NATIONAL LABORATORIES , HEALTH AND SAFETY DIVISION",///,25X,"*
     5**MATHEMATICAL MODELING OF AQUATIC DISPERSION OF EFFLUENTS ***")
      WRITE(6,4)
    4 FORMAT(//10X,"THE PROGRAM IS LAST UPDATED ON JUNE 26, 1980")
      WRITE(6,5) ISEC,ITIME,NNBC,NDBC,NMBC,IGAMG
    5 FORMAT(//,10X,"ISEC = ",I3,2X,"ITIME = ",I3,2X,"NNBC =",I3,2X,"NDBC =
     2C =",I3,2X,"NMBC =",I3,2X,"IGAMG = ",I3/)
      CALL INP
  128 CONTINUE
      DO 10 J=1,3
      DO 10 I=1,1000
      P(I,J) = 0.
      S(I,J) = 0.
   10 R(I) = 0.
      DO 20 II=1,NELEM
      AL = X(II+1) - X(II)
      JJ = II+ 1
      KK = II  - 1
      IF(KK.EQ.0) KK = II
      IF(JJ.GT.NELEM) JJ = NELEM
      DXX = DX(II)
      UU = U(II)
      FF = GAMA(II)
      GG = G(II)
      DX1 = (DX(II) + DX(KK))/2.
      DX2 = (DX(II)  + DX(JJ))/2.
      U1 = (U(II) + U(KK))/2.
      U2 = (U(II) + U(JJ))/2.
      F1 = (GAMA(II) + GAMA(KK))/2.
      F2 = (GAMA(II) + GAMA(JJ))/2.
      G1 = (G(II) + G(KK))/2.
      G2 = (G(II) + G(JJ))/2.
      IF(ISEC.EQ.1) CALL EL2N1
      IF(ISEC.EQ.2) CALL EL2N2
      IF(ISEC.EQ.3) CALL EL2N3
      IF(ISEC.EQ.4) CALL EL2N4
      IF(ISEC.EQ.5) CALL EL2N5
   18 CONTINUE
      IF(ITIME.EQ.1) CALL MASS
      CALL ASSEM
   20 CONTINUE
      IF(ITIME.EQ.1) GO TO 50
```

```
      DO 51 I=1,NNODE
 51   RBN(I)=R(I)
      DO 52 I=1,NNODE
      DO 52 J=1,3
 52   CC(I,J) = S(I,J)
      CALL BOUND(CC,RBN)
      CALL REDUCE(CC,R)
      CALL SOLVE(CC,R)
      DO 53 I=1,NNODE
      CIN(I)=R(I)
 53   R(I) = RBN(I)
      CALL OUT
      GO TO 100
 50   CONTINUE
      TCONT = TI + TST
      DO 122 I=1,NNODE
      DO 122 J=1,3
122   P(I,J) = ((P(I,J)*2./TST) - S(I,J))
      DO 123 I=1,NNODE
      DO 123 J=1,3
123   S(I,J) = (P(I,J) + 2.*S(I,J))
124   CONTINUE
      DO 126 IT=1,IP
      CALL MLTPLY(P,CIN,RBN)
      DO 125 I=1,NNODE
125   RBN(I) = 2.*R(I) + RBN(I)
      DO 777 I=1,NNODE
      DO 777 J=1,3
777   CC(I,J) = S(I,J)
      IF(TCONT.LT.TD) GO TO 778
      NNBC = 0
      NDBC = 1
      NMBC = 0
      BCD(1)=0.
778   CONTINUE
      CALL BOUND(CC,RBN)
      CALL REDUCE(CC,RBN)
      CALL SOLVE(CC,RBN)
      DO 776 I=1,NNODE
776   CIN(I) = RBN(I)
      IF(IT.EQ.IP) GO TO 127
126   TCONT = TCONT + TST
127   CONTINUE
      CALL OUT
      TCONT = TCONT + TST
      IF(TCONT - TF) 124,124,130
130   CONTINUE
100   CONTINUE
      WRITE(6,101) TITLE
101   FORMAT(//20X,"END OF THE PROBLEM",20X,18A4)
      STOP
      END
      SUBROUTINE BOUND(CC,RBN)
      COMMON/BC/NBCN,BCN,NDBCN,BCD,NMBCN,BCM
      COMMON/CONS/ISEC,ITIME,IDXGEN,NNBC,NDBC,NMBC,IP,IGAMG,IUNIT
      COMMON/GMV/S,R,P,CIN
      DIMENSION S(1000,3),R(1000),P(1000,3),CIN(1000),CC(1000,3),
     2RBN(1000),NBCN(5),BCN(5),NDBCN(5),BCD(5),NMBCN(5),BCM(5)
      IF(ITIME.EQ.1) GO TO 100
      IF(NDBC.EQ.0) GO TO 101
      DO 1 I=1,NDBC
      NK = NDBCN(I)
      CC(NK,2) = CC(NK,2) * 10.**25
      R(NK) = R(NK) + CC(NK,2)*BCD(I)
  1   CONTINUE
      GO TO 101
100   CONTINUE
      IF(NDBC.EQ.0) GO TO 101
```

```
      DO 2 I=1,NDBC
      NK = NDBCN(I)
      CC(NK,2) = CC(NK,2) * 10.**25
      RBN(NK) = RBN(NK) + CC(NK,2)*BCD(I)
    2 CONTINUE
  101 CONTINUE
      IF(NNBC.EQ.0) GO TO 102
      DO 3 I=1,NNBC
      NK = NBCN(I)
    3 RBN(NK) = RBN(NK) + BCN(I)
  102 CONTINUE
      IF(NMBC.EQ.0) GO TO 103
      DO 4 I=1,NMBC
      NK = NMBCN(I)
    4 CC(NK,2) = CC(NK,2) + BCM(I)
  103 CONTINUE
      RETURN
      END
      SUBROUTINE MASS
      COMMON/MVEL/ SE,RE,PE,AL,II
      DIMENSION SE(2,2),RE(2),PE(2,2)
      PE(1,1) = AL/3.
      PE(1,2) = AL/6.
      PE(2,1) = PE(1,2)
      PE(2,2) = PE(1,1)
      RETURN
      END
      SUBROUTINE INP
      COMMON TITLE,TI,TF,TST,TCONT,TD
      COMMON/BC/NBCN,BCN,NDBCN,BCD,NMBCN,BCM
      COMMON/CONS/ISEC,ITIME,IDXGEN,NNBC,NDBC,NMBC,IP,IGAMG,IUNIT
      COMMON/DATA/DX,U,GAMA,X,G
      COMMON/GMV/S,R,P,CIN
      COMMON/CHR/NNODE,NELEM,MAT
      DIMENSION DX(1000),U(1000),GAMA(1000),X(1000),G(1000)
     2,NBCN(5),BCN(5),NDBCN(5),BCD(5),NMBCN(5),BCM(5),
     3S(1000,3),R(1000),P(1000,3),CIN(1000),TITLE(20)
      READ(5,1) TITLE
    1 FORMAT(20A4,F8.0)
      WRITE(6,2) TITLE
    2 FORMAT(1H1,10X,20A4//)
      READ(5,3) NCNP,NCEL
    3 FORMAT(2I5)
      WRITE(6,4) NCNP,NCEL
    4 FORMAT(/10X,"NCNP = ",I3,5X,"NCEL = ",I3//)
      WRITE(6,5)
    5 FORMAT(/,10X,"GENERATED DATA FOR THE PROBLEM"//,10X,
     2"NODAL POINTS AND NODAL COORDINATES"//)
      NCN = 0
    5 NCN=NCN+1
      IF(NCN.GT.NCNP) GO TO 15
      READ(5,10) N,X(N),NMIS
   10 FORMAT(I10,F10.4,I10)
      WRITE(6,11) N,X(N)
   11 FORMAT(1H ,13X,4HNODE,I4,5X,3HX= ,F10.4)
      NI=N
      IF(NMIS.EQ.0) GO TO 9
   12 NCN=NCN + 1
      IF(NCN.GT.NCNP) GO TO 15
      READ(5,10) N,X(N),NMIS
      NE = N
      NPG = NE - NI
      DXD = (X(NE) - X(NI))/FLOAT(NPG)
      DO 13 IJ=1,NPG
      I = IJ
      NG = NI + I
      X(NG) = X(NI) + FLOAT(I)*DXD
   13 WRITE(6,11) NG,X(NG)
```

```
      IF(NMIS.EQ.0) GO TO 9
      NI = N
      GO TO 12
   15 NNODE = N
      IF(NNODE.LE.1000) GO TO 14
      WRITE(6,16)
   16 FORMAT(1H1,"ERROR*** NUMBER OF NODES GREATER THAN 1000,")
      GO TO 4000
   14 N=0
      DO 19 M=1,NCEL
      N=N+1
      READ(5,17) NMIS,U(N),GAMA(N),G(N),IDXGEN,DX(N)
   17 FORMAT(I5,3F10.4,I5,F10.4)
      IF(IDXGEN.GT.0) CALL DIFF(N)
      DO 18 K=1,NMIS
      N=N+1
      DX(N)=DX(N-1)
      GAMA(N)=GAMA(N-1)
      U(N)=U(N-1)
      G(N)=G(N-1)
   18 CONTINUE
   19 CONTINUE
      NELEM=N
      IF(NELEM.LE.999) GO TO 21
      WRITE(6,20)
   20 FORMAT(1H1,"ERROR**** NUMBER OF ELEMENTS GREATER THAN 999",2X,
     2"CHANGE DIMENSIONS OF THE PROGRAM"/)
   21 CONTINUE
      WRITE(6,22) NNODE,NELEM
   22 FORMAT(1H1,//,11X,"NUMBER OF NODES = ",I5,3X//8X,
     2"NUMBER OF ELEMENTS = ",I5,///25X," E L E M E N T   D A T A "//)
      IF(IGAMG.EQ.1) WRITE(6,669)
  669 FORMAT(10X,"NOTE** IN THIS PROBLEM DECAY CONSTANT IS GENERATED:
     2  THUS DECAY CONSTANT LISTED BELOW SHOULD BE IGNORED"//)
      WRITE(6,8)
    8 FORMAT(1X,"ELEM. NO:",1X,"NODE 1",1X,"NODE 2",1X,"VELOCITY 1",1X,
     2"VELOCITY 2",1X,"VELOCITY",1X,"DIFF. COEF. 1",1X,"DIFF. COEF. 2",
     31X,"DIFF. COEF.",1X,"DECAY 1",1X,"DECAY 2",1X,"DECAY CONS.",1X,
     4"LOAD FUNC"/)
      DO 23 NJ=1,NELEM
      N=NJ
      M=N+1
      MM=M
      IF(M.GT.NELEM) M=NELEM
      IF(ISEC.EQ.1) WRITE(6,24) N,N,MM,U(N),DX(N),GAMA(N),G(N)
   24 FORMAT(I9,I8,I7,21X,F10.4,28X,F10.4,19X,F10.5,F10.4)
      IF(ISEC.EQ.2) WRITE(6,25) N,N,MM,U(N),U(M),DX(N),DX(M),GAMA(N),
     2GAMA(M),G(N)
   25 FORMAT(I9,I8,I7,1X,F10.4,F10.4,11X,F12.4,F13.4,11X,F10.4,F9.4,10X
     2,F10.4)
      IF(ISEC.EQ.3) WRITE(6,26) N,N,MM,U(N),U(M),DX(N),GAMA(N),G(N)
   26 FORMAT(I9,I8,I7,1X,F10.4,F10.4,39X,F10.4,14X,F13.5,F10.4)
      IF(ISEC.EQ.4) WRITE(6,49) N,N,MM,U(N),U(M),DX(N),GAMA(N),GAMA(M),
     2G(N)
   49 FORMAT(I9,I8,I7,1X,F10.4,F10.4,37X,F10.4,F10.4,F9.4,10X,F10.4)
      IF(ISEC.EQ.5) WRITE(6,50) N,N,MM,U(N),U(M),DX(N),DX(M),GAMA(N),
     2G(N)
   50 FORMAT(I9,I8,I7,1X,F10.4,F10.4,11X,F12.4,F13.4,28X,F10.5,F12.4)
   23 CONTINUE
      IF(ITIME.EQ.0) GO TO 36
      READ(5,27) TI,TF,TST,TD,IP
      WRITE(6,28)
      WRITE(6,29) TI,TF,TST,TD
   27 FORMAT(4F10.0,I10)
   28 FORMAT(///,10X,"TIME DEPENDENT DATA")
   29 FORMAT(/,5X,"INITIAL TIME =",E12.6,5X,"FINAL TIME =",E12.6,5X,"TIM
     2E STEP =",E12.6,5X,"CONCENTRATION DURATION =",E12.6)
      N=0
```

```
 777 CONTINUE
     N=N+1
     IF(N.GT.NNODE) GO TO 32
     READ(5,30) NMIS,CIN(N)
  30 FORMAT(I10,F10.0)
     IF(NMIS.EQ.0) GO TO 777
     DO 31 K=1,NMIS
     N=N+1
     CIN(N)=CIN(N-1)
  31 CONTINUE
     IF(N.LT.NNODE) GO TO 777
  32 CONTINUE
     WRITE(6,33)
     WRITE(6,34)
  33 FORMAT(//,10X,"INITIAL VALUES OF CONCENTRATION"//)
  34 FORMAT(//4(5X,"I",4X,"CIN(I)",10X))
     WRITE(6,35) ((I,CIN(I)),I=1,NNODE)
  36 CONTINUE
  35 FORMAT(4(I6,E20.10))
     IF(IGAMG.EQ.0) GO TO 771
     READ(5,3) MAT,IUNIT
     IF(IUNIT.EQ.1) WRITE(6,801) MAT
     IF(IUNIT.EQ.2) WRITE(6,802) MAT
     IF(IUNIT.EQ.3) WRITE(6,803) MAT
     IF(IUNIT.EQ.4) WRITE(6,804) MAT
 801 FORMAT(//10X,"UNIT OF TIME FOR DECAY CONSTANT IS CHOSEN AS SECONDS
    2",2X,"MATERIAL NUMBER IS CHOSEN AS =" ,I5//)
 802 FORMAT(//10X,"UNIT OF TIME FOR DECAY CONSTANT IS CHOSEN AS MINUTES
    2",2X,"MATERIAL NUMBER IS CHOSEN AS =" ,I5//)
 803 FORMAT(//10X,"UNIT OF TIME FOR DECAY CONSTANT IS CHOSEN AS HOURS"
    2,2X,"MATERIAL NUMBER IS CHOSEN AS =" ,I5//)
 804 FORMAT(//10X,"UNIT OF TIME FOR DECAY CONSTANT IS CHOSEN AS DAYS"
    2,2X,"MATERIAL NUMBER IS CHOSEN AS =" ,I5//)
     CALL GAMGEN
 771 CONTINUE
     IF(NNBC.EQ.0) GO TO 90
     DO 37 I=1,NNBC
  37 READ(5,38) NBCN(I),BCN(I)
  90 CONTINUE
  38 FORMAT(I10,F10.0)
     IF(NDBC.EQ.0) GO TO 91
     DO 39 I=1,NDBC
  39 READ(5,38) NDBCN(I),BCD(I)
  91 CONTINUE
     IF(NMBC.EQ.0) GO TO 92
     DO 40 I=1,NMBC
  40 READ(5,38) NMBCN(I),BCM(I)
  92 CONTINUE
     DO 41 I=1,NNBC
  41 WRITE(6,42) NBCN(I),BCN(I)
  42 FORMAT(//6X,"NEUMAN NODE =",I5,8X,"NEUMAN B.C. =",F12.6)
     DO 43 I=1,NDBC
  43 WRITE(6,44) NDBCN(I),BCD(I)
  44 FORMAT(//3X,"DIRICHLET NODE =",I5,5X,"DIRICHLET B.C. =",F12.6)
     DO 45 I=1,NMBC
  45 WRITE(6,46) NMBCN(I),BCM(I)
  46 FORMAT(//2X,"MIXED B.C. NODE =",I5,9X,"MIXED B.C. =",F12.6////)
4000 CONTINUE
     RETURN
     END
     SUBROUTINE ASSEM
     COMMON/CHR/ NNODE,NELEM,MAT
     COMMON/MVEL/ SE,RE,PE,AL,II
     COMMON/GMV/ S,R,P,CIN
     DIMENSION SE(2,2),RE(2),PE(2,2),S(1000,3),R(1000),P(1000,3)
    2,CIN(1000)
C**DOES NOT HANDLE RIVER BRANCHES. NODAL PATTERN SHOULD BE READ IN*
     S(II,2) = S(II,2) + SE(1,1)
```

```
      S(II,3) = S(II,3) + SE(1,2)
      S(II+1,1) = S(II+1,1) + SE(2,1)
      S(II+1,2) = S(II+1,2) + SE(2,2)
      P(II,2) = P(II,2) + PE(1,1)
      P(II,3) = P(II,3) + PE(1,2)
      P(II+1,1) = P(II+1,1) + PE(2,1)
      P(II+1,2) = P(II+1,2) + PE(2,2)
      R(II) = R(II) + RE(1)
      R(II+1) = R(II+1) + RE(2)
      RETURN
      END
      SUBROUTINE EL2N1
      COMMON/ELM/DXX,UU,FF,U1,U2,DX1,DX2,F1,F2,GG,G1,G2
      COMMON/MVEL/ SE,RE,PE,AL,II
      DIMENSION SE(2,2),RE(2),PE(2,2)
      SE(1,1) = (DXX/AL) - (UU/2.) + (FF*AL/3.)
      SE(1,2) = (UU/2.) - (DXX/AL) + (FF*AL/6.)
      SE(2,1) = (-(UU/2.)) - (DXX/AL) + (FF*AL/6.)
      SE(2,2) = (DXX/AL) + (UU/2.) + (FF*AL/3.)
      RE(1) = GG*AL/2.
      RE(2) = GG*AL/2.
      RETURN
      END
      SUBROUTINE EL2N2
      COMMON/ELM/DXX,UU,FF,U1,U2,DX1,DX2,F1,F2,GG,G1,G2
      COMMON/MVEL/ SE,RE,PE,AL,II
      DIMENSION SE(2,2),RE(2),PE(2,2)
      SE(1,1) = (DX1/(2.*AL)) - (U1/3.) + (F1*AL/4.)-(U2/6.)+(F2*AL/12.)
     2 + (DX2/(2.*AL))
      SE(1,2) =-(DX2/(2.*AL))+(U2/6.)+(F2*AL/12.)+(U1/3.)+(F1*AL/12.)
     2 - (DX1/(2.*AL))
      SE(2,1) =-(DX1/(2.*AL))-(U1/6.)+(F1*AL/12.)-(U2/3.)+(F2*AL/12.)
     2 - (DX2/(2.*AL))
      SE(2,2) = (DX2/(2.*AL))+(U2/3.)+(F2*AL/4.)+(U1/6.)+(F1*AL/12.)
     2 + (DX1/(2.*AL))
      RE(1) = G1*AL/3. + G2*AL/6.
      RE(2) = G1*AL/6. + G2*AL/3.
      RETURN
      END
      SUBROUTINE EL2N3
      COMMON/ELM/DXX,UU,FF,U1,U2,DX1,DX2,F1,F2,GG,G1,G2
      COMMON/MVEL/ SE,RE,PE,AL,II
      DIMENSION SE(2,2),RE(2),PE(2,2)
      SE(1,1) = (DXX/AL) - (U1/3.) - (U2/6.) + (FF*AL/3.)
      SE(1,2) =-(DXX/AL) + (U2/6.) + (U1/3.) + (FF*AL/6.)
      SE(2,1) =-(DXX/AL) - (U1/6.) - (U2/3.) + (FF*AL/6.)
      SE(2,2) = (DXX/AL) + (U2/3.) + (U1/6.) + (FF*AL/3.)
      RE(1) = G1*AL/3. + G2*AL/6.
      RE(2) = G1*AL/6. + G2*AL/3.
      RETURN
      END
      SUBROUTINE EL2N4
      COMMON/ELM/DXX,UU,FF,U1,U2,DX1,DX2,F1,F2,GG,G1,G2
      COMMON/MVEL/ SE,RE,PE,AL,II
      DIMENSION SE(2,2),RE(2),PE(2,2)
      SE(1,1) = (DXX/AL)-(U1/3.)+(F1*AL/4.)-(U2/6.)+(F1*AL/12.)
      SE(1,2) =-(DXX/AL)+(U2/6.)+(F2*AL/12.)+(U1/3.)+(F1*AL/12.)
      SE(2,1) =-(DXX/AL)-(U1/6.)+(F1*AL/12.)-(U2/3.)+(F2*AL/12.)
      SE(2,2) = (DXX/AL)+(U2/3.)+(F2*AL/4.)+(U1/6.)+(F1*AL/12.)
      RE(1) = G1*AL/3. + G2*AL/6.
      RE(2) = G1*AL/6. + G2*AL/3.
      RETURN
      END
      SUBROUTINE EL2N5
      COMMON/ELM/DXX,UU,FF,U1,U2,DX1,DX2,F1,F2,GG,G1,G2
      COMMON/MVEL/ SE,RE,PE,AL,II
      DIMENSION SE(2,2),RE(2),PE(2,2)
      SE(1,1) = (DX1/(2.*AL)) - (U1/3.) - (U2/6.) + (FF*AL/3.)
```

```
  2 + (DX2/(2.*AL))
    SE(1,2) =-(DX2/(2.*AL)) + (U2/6.) + (U1/3.) + (FF*AL/6.)
  2 - (DX1/(2.*AL))
    SE(2,1) =-(DX1/(2.*AL)) - (U1/6.) - (U2/3.) + (FF*AL/6.)
  2 - (DX2/(2.*AL))
    SE(2,2) = (DX2/(2.*AL)) + (U2/3.) + (U1/6.) + (FF*AL/3.)
  2 + (DX1/(2.*AL))
    RE(1) = G1*AL/3. + G2*AL/6.
    RE(2) = G1*AL/6. + G2*AL/3.
    RETURN
    END
    SUBROUTINE OUT
    COMMON TITLE,TI,TF,TST,TCONT,TD
    COMMON/CHR/ NNODE,NELEM,MAT
    COMMON/CONS/ISEC,ITIME,IDXGEN,NNBC,NDBC,NMBC,IP,IGAMG,IUNIT
    COMMON/GMV/S,R,P,CIN
    DIMENSION S(1000,3),R(1000),P(1000,3),CIN(1000),TITLE(20)
    IF(ITIME.EQ.0) GO TO 10
    WRITE(6,1)
  1 FORMAT(/20X,"RESULTS OF THE TIME DEPENDENT PROBLEM"//)
    WRITE(6,2) TCONT
  2 FORMAT(10X,"VALUES OF CONCENTRATION AT TIME = ",E12.5//
   2,4(5X,"I",14X" C(I) "))
    WRITE(6,5) ((I,CIN(I)),I=1,NNODE)
  5 FORMAT(4(I6,E20.10))
    GO TO 20
 10 CONTINUE
    WRITE(6,3)
  3 FORMAT(/20X,"RESULTS OF THE STEADY STATE PROBLEM")
    WRITE(6,4)
  4 FORMAT(10X,"VALUES OF THE STEADY STATE CONCENTRATION"//
   2,4(5X,"I",14X," C(I)"))
    WRITE(6,5) ((I,CIN(I)),I=1,NNODE)
 20 CONTINUE
    RETURN
    END
    SUBROUTINE REDUCE(A,B)
    COMMON/CHR/ NTDOF,NELEM,MAT
    DIMENSION A(1000,3),B(1000)
    DO 1 N=1,NTDOF
    LL=2
    I=N+1
    IF(I.GT.NTDOF) GO TO 1
    LL= LL-1
    IF(A(I,LL).EQ.0.) GO TO 2
    C=A(I,LL)/A(N,2)
    J=LL+1
    A(I,J) = A(I,J) - C*A(N,3)
    B(I) = B(I) - C * B(N)
  2 CONTINUE
  1 CONTINUE
    RETURN
    END
    SUBROUTINE SOLVE(A,B)
    COMMON/CHR/NTDOF,NELEM,MAT
    DIMENSION A(1000,3),B(1000)
    B(NTDOF) = B(NTDOF)/A(NTDOF,2)
    DO 1 M=2,NTDOF
    N=NTDOF +1-M
    IF(A(N,3).EQ.0.) GO TO 4
    K = N + 1
    IF(K.GT.NTDOF) GO TO 1
    B(N) = B(N) - A(N,3) * B(K)
  4 CONTINUE
    B(N) = B(N)/A(N,2)
  1 CONTINUE
    RETURN
    END
```

```
      SUBROUTINE MLTPLY(S,PHI,F)
      COMMON/CHR/NTDOF,NELEM,MAT
      DIMENSION S(1000,3),PHI(1000),F(1000)
      DO 1 I=1,NTDOF
    1 F(I) = 0.
      K = 3
      DO 2 I=1,2
      K = K - 1
      L = 1
      DO 2 J=K,3
      F(I) = F(I) + S(I,J)*PHI(L)
      L = L + 1
    2 CONTINUE
      K = 1
      MID = NTDOF - 2
      DO 3 I=3,MID
      K = K + 1
      L = K
      DO 3 J=1,3
      F(I) = F(I) + S(I,J) * PHI(L)
      L = L + 1
    3 CONTINUE
      K = NTDOF - 3
      JJ = 4
      NREST = NTDOF - 1
      DO 4 I=NREST,NTDOF
      JJ = JJ - 1
      K = K + 1
      L = K
      DO 4 J=1,JJ
      F(I) = F(I) + S(I,J) * PHI(L)
      L = L + 1
    4 CONTINUE
      RETURN
      END
      SUBROUTINE GAMGEN
      COMMON TITLE,TI,TF,TST,TCONT,TD
      COMMON/DATA/DX,U,GAMA,X,G
      COMMON/CONS/ISEC,ITIME,IDXGEN,NNBC,NDBC,NMBC,IP,IGAMG,IUNIT
      COMMON/CHR/NNODE,NELEM,MAT
      DIMENSION DX(1000),U(1000),GAMA(1000),X(1000),G(1000),TITLE(20)
     2,HLF(63)
      DATA HLF/12.3,5730.,2.58,0.00171,0.0391,0.241,0.23,0.076,0.857,
     22.7,.123,.756,.194,5.26,92.,.00146,.668,.0016,.0512,.138,28.5
     3,.176,.0265,.161,.00114,.172,.096,.0019,.00753,.112,.00405,
     41.,.739,.00767,.165,.026,2.7,.159,.0106,.3,.00106,.0904,
     5.00144,.00342,.022,.0088,.0024,2.1,.00076,.0356,30.,.0351,.0046,
     6.0877,.0036,.0237,.795,.031,2.6,.315,.202,.0027,.0063/
      IF(IUNIT.EQ.1) HLFL=HLF(MAT)*31536000.
      IF(IUNIT.EQ.2) HLFL=HLF(MAT)*525600.
      IF(IUNIT.EQ.3) HLFL=HLF(MAT)*8760.
      IF(IUNIT.EQ.4) HLFL=HLF(MAT)*365.
      DO 2 I=1,NNODE
      GAMA(I)= (0.693147/HLFL)
    2 CONTINUE
      WRITE(6,3) GAMA(1)
    3 FORMAT(///10X,"DECAY CONSTANT GENERATED FOR THIS PROBLEM IS = "
     2 ,E12.6//)
      RETURN
      END
      SUBROUTINE DIFF(N)
      COMMON/CONS/ISEC,ITIME,IDXGEN,NNBC,NDBC,NMBC,IP,IGAMG,IUNIT
      COMMON/DATA/DX,U,GAMA,X,G
      COMMON/CHR/ NNODE,NELEM,MAT
      DIMENSION DX(1000),U(1000),GAMA(1000),X(1000),G(1000)
      IF(IDXGEN.EQ.2) GO TO 10
      IF(IDXGEN.EQ.3) GO TO 20
      READ(5,2) W,DEP,US
```

```
  2 FORMAT(4F10.3)
    DX(N)=(0.011*(U(N)**2.)*(W**2.))/(DEP*US)
    GO TO 30
 10 READ(5,2) Q,R,US
    BET = 0.18*(US/U(N))**1.5
    DX(N) = (BET*(Q**2.))/(US*R**3.)
    GO TO 30
 20 CONTINUE
    READ(5,2) Q,R,US,ALR
    DX(N)=.0019*((US/U(N))**.25)*(ALR**4.56)*((Q**2.)/(US*R**3))
 30 CONTINUE
    RETURN
    END
```